

Supporting Information

The Dual-Phase Mechanism for the Catalytic Conversion of *n*-Butane to Maleic Anhydride by the Vanadyl Pyrophosphate (VPO) Heterogeneous Catalyst

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1. Modified basis set, mod-LACVP**

We present mod-LACVP** in Gaussian94 format. We indicate Gaussians removed from LACVP** to form mod-LACVP** using strikethrough.

1.1 Hydrogen

S	3	1.00	
		18.7311370	0.03349460
		2.8253937	0.23472695
		0.6401217	0.81375733
S	1	1.00	
		0.1612778	1.0000000
P	1	1.00	
		1.1000000	1.0000000

1.2 Carbon

S	6	1.00	
		3047.5249000	0.0018347
		457.3695100	0.0140373
		103.9486900	0.0688426
		29.2101550	0.2321844
		9.2866630	0.4679413
		3.1639270	0.3623120
SP	3	1.00	
		7.8682724	-0.1193324 0.0689991
		1.8812885	-0.1608542 0.3164240
		0.5442493	1.1434564 0.7443083
SP	1	1.00	
		0.1687144	1.0000000 1.0000000
D	1	1.00	
		0.8000000	1.0000000

1.3 Oxygen

S	6	1.00	
		5484.6717000	0.0018311
		825.2349500	0.0139501
		188.0469600	0.0684451
		52.9645000	0.2327143
		16.8975700	0.4701930
		5.7996353	0.3585209
SP	3	1.00	
		15.5396160	-0.1107775 0.0708743
		3.5999336	-0.1480263 0.3397528

	1.0137618	1.1307670	0.7271586
SP 1	1.00		
	0.2700058	1.0000000	1.0000000
D 1	1.00		
	0.8000000	1.0000000	

1.4 Phosphorus

S 6	1.00		
	19413.3000000	0.0018516	
	2909.4200000	0.0142062	
	661.3640000	0.0699995	
	185.7590000	0.2400790	
	59.1943000	0.4847620	
	20.0310000	0.3352000	
SP 6	1.00		
	339.4780000	-0.00278217	0.00456462
	81.0101000	-0.0360499	0.03369360
	25.8780000	-0.1166310	0.13975500
	9.4522100	0.0968328	0.33936200
	3.6656600	0.6144180	0.45092100
	1.4674600	0.4037980	0.23858600
SP 3	1.00		
	2.1562300	-0.2529230	-0.01776530
	0.7489970	0.0328517	0.27405800
	0.2831450	1.0812500	0.78542100
SP 1	1.00		
	0.0998317	1.0000000	1.00000000
D 1	1.00		
	0.5500000	1.0000000	

1.5 Vanadium (diffuse functions needed to be removed)

S 3	1.00		
	4.5900000	-0.4277302	
	1.4930000	0.7069691	
	0.5570000	0.5895813	
S 4	1.00		
	4.5900000	0.2501081	
	1.4930000	-0.4697777	
	0.5570000	-0.7129415	
	0.0975000	1.1006569	
S 1	1.00		
	0.0342000	1.0000000	
P 3	1.00		
	13.7600000	-0.0482312	

	1.7120000	0.6141161
	0.5587000	0.4838342
P 1 1.00	0.0590000	1.0000000
P 1 1.00	0.0180000	1.0000000
D 4 1.00	25.7000000	0.0331033
	6.5300000	0.1795753
	2.0780000	0.4373062
	0.6243000	0.5984860
D 1 1.00	0.1542000	1.0000000
ECP		
d-ul potential		
3		
1	296.4487582	-10.0000000
2	53.5015052	-54.8909808
2	13.3204510	-9.7010586
s-ul potential		
5		
0	93.2193654	3.0000000
1	71.1029567	22.5345689
2	33.8766993	216.5634009
2	6.8691200	252.6822538
2	6.4804722	-176.2671654
p-ul potential		
5		
0	52.0953977	5.0000000
1	65.6778411	5.7003555
2	27.4703764	182.9054274
2	6.2352020	117.2756226
2	5.8139909	-78.5829134

2. X1-based mechanism and calculated enthalpies

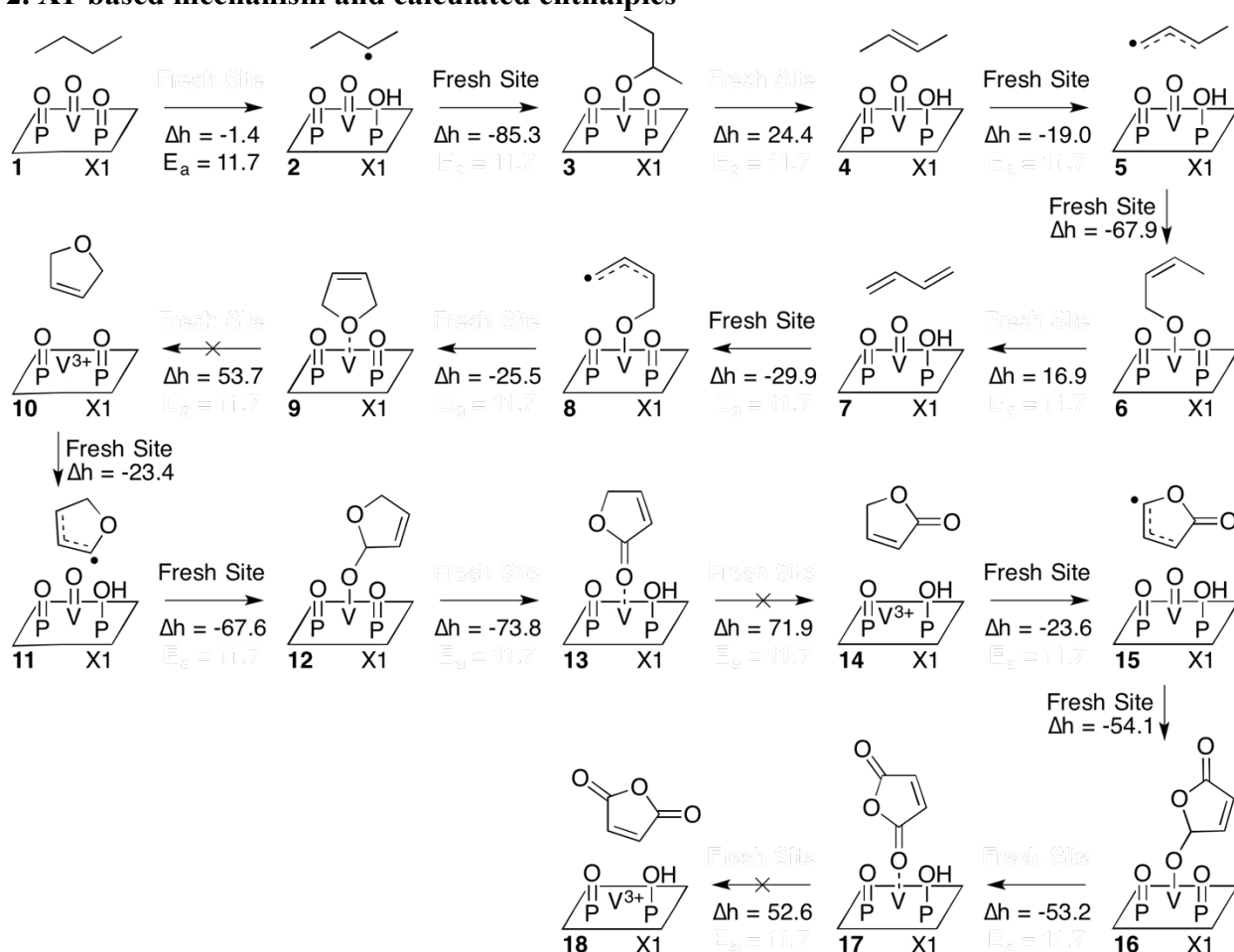


Figure S1. B3LYP-derived mechanism for the gas phase conversion of *n*-butane to MA entirely on the X1 phase, with reaction enthalpies and barriers in kcal/mol. Many steps, particularly adsorptions, are too exothermic to be compatible with VPO's high observed selectivity. Additionally, desorption steps are far too endothermic to occur under catalytic conditions.

3. Atomic coordinates and ground state energies

3.1 Finite Clusters

Due to the sheer quantity of optimized structures (one for each functional/basis set combination), we only provide initial structures.

P₄O₁₀

PBE/LACVP** Energy: -2116.539596 Ha

M06/LACVP** Energy: -2117.570139 Ha

B3LYP/LACVP** Energy: -2117.945784 Ha

B3LYP/LACV3P** Energy: -2118.271433 Ha

B3LYP/mod-LACVP** Energy: -2117.945784 Ha

P1	3.72463700000000	3.19939800000000	2.45186300000000
P2	1.42559900000000	3.64191300000000	3.82883800000000
P3	2.93400300000000	1.44964400000000	4.37298400000000
P4	1.56333600000000	1.60845100000000	2.03341800000000
O5	1.93452500000000	2.62073300000000	5.08280500000000
O6	4.29884500000000	2.16565200000000	3.66673100000000
O7	2.74761100000000	4.42016700000000	3.10714100000000
O8	2.07617700000000	0.52954200000000	3.23641600000000
O9	2.88926100000000	2.32897700000000	1.26074200000000
O10	0.52494300000000	2.78405400000000	2.67681600000000
O11	4.92069900000000	3.85955800000000	1.79594900000000
O12	3.40970300000000	0.51554200000000	5.46740700000000
O13	0.52697600000000	4.70525300000000	4.42748900000000
O14	0.79020400000000	0.81903700000000	0.99626100000000

P₄O₁₀H (POH)

PBE/LACVP** Energy: -2117.075853 Ha

M06/LACVP** Energy: -2118.100811 Ha

B3LYP/LACVP** Energy: -2118.485104 Ha

B3LYP/LACV3P** Energy: -2118.813951 Ha

B3LYP/mod-LACVP** Energy: -2118.485104 Ha

P1	3.80667900000000	3.24487300000000	2.40610900000000
P2	1.36471800000000	3.71453700000000	3.86999800000000
P3	2.96625600000000	1.38605800000000	4.44800900000000
P4	1.51109700000000	1.55454700000000	1.96256900000000
O5	1.97948200000000	2.60785400000000	4.90579100000000
O6	4.12268400000000	2.19425800000000	3.61985100000000
O7	2.71652300000000	4.23960700000000	3.11311300000000
O8	2.10725200000000	0.71084500000000	3.23074400000000
O9	2.84439700000000	2.34320300000000	1.43764300000000
O10	0.70110200000000	2.75482300000000	2.72354900000000
O11	4.95428800000000	3.87870700000000	1.77612200000000
O12	3.42192200000000	0.48811600000000	5.49841100000000

O13	0.5014220000000	4.7348950000000	4.4453260000000
O14	0.7687640000000	0.7956660000000	0.9673790000000
H15	5.7897090000000	3.3485590000000	1.8497500000000

P₄O₁₀H (P-OH-P)

PBE/LACVP** Energy: -2117.080009 Ha

M06/LACVP** Energy: -2118.10728 Ha

B3LYP/LACVP** Energy: -2118.494147 Ha

B3LYP/LACV3P** Energy: -2118.808393 Ha

B3LYP/mod-LACVP** Energy: -2118.494147 Ha

P1	3.8448745613662	2.9387018077079	2.3729943021733
P2	1.4943564043802	3.6263066651119	3.7463337140718
P3	2.9252096114034	1.3150518346126	4.4488874850898
P4	1.5170024467387	1.4084274637531	2.0217349656798
O5	2.0238608115538	2.5832505452359	4.8486820163573
O6	4.1231424427581	1.9776661954511	3.6212022294324
O7	2.8490476359940	4.0399754053950	2.9862918276671
O8	2.0501528263297	0.6023695115319	3.3057734419129
O9	2.8727316300267	2.0545087982765	1.4492499173537
O10	0.7654436337737	2.6710598812973	2.6764267913307
O11	5.0716339033409	3.4600719995696	1.7088719289001
O12	3.3601192057914	0.4388782731084	5.5717373901619
O13	0.6674798599229	4.7567179306333	4.2642603276215
O14	0.7142379252550	0.6143016370022	1.0450460837450
H15	4.8482763943332	1.3882831702752	3.4814494446396

VP₃O₁₀

PBE/LACVP** Energy: -1846.804745 Ha

M06/LACVP** Energy: -1847.622022 Ha

B3LYP/LACVP** Energy: -1848.002446 Ha

B3LYP/LACV3P** Energy: -1848.316212 Ha

B3LYP/mod-LACVP** Energy: -1847.989994 Ha

P1	3.7647920000000	3.2282720000000	2.4597990000000
P2	1.4220390000000	3.6793400000000	3.8604670000000
P3	2.9580440000000	1.4465310000000	4.4164270000000
V4	1.4966830000000	1.5391350000000	1.9423300000000
O5	1.9134240000000	2.6085550000000	5.0859400000000
O6	4.3065540000000	2.1477950000000	3.6551490000000
O7	2.7375060000000	4.4286170000000	3.0872120000000
O8	2.1347500000000	0.3905900000000	3.3795150000000
O9	3.0504970000000	2.4128530000000	1.1586830000000
O10	0.3913780000000	2.9248840000000	2.7484540000000
O11	4.9902000000000	3.9363120000000	1.9177410000000
O12	3.4855390000000	0.6131240000000	5.5670690000000
O13	0.6207170000000	4.7775920000000	4.5301730000000
O14	0.4943960000000	0.5143230000000	0.5958990000000

VP₃O₁₀H (POH)

PBE/LACVP** Energy: -1847.399548 Ha

M06/LACVP** Energy: -1848.237437 Ha

B3LYP/LACVP** Energy: -1848.632631 Ha

B3LYP/LACV3P** Energy: -1848.952959 Ha

B3LYP/mod-LACVP** Energy: -1848.618964 Ha

P1	-0.995700000000	-0.484332000000	-1.460527000000
P2	1.454504000000	-1.114956000000	-0.000001000000
P3	-0.995654000000	-0.484084000000	1.460543000000
V4	0.430063000000	1.665190000000	-0.000035000000
O5	0.429958000000	-1.268266000000	1.268999000000
O6	-1.699091000000	-0.720655000000	-0.000001000000
O7	0.429942000000	-1.268245000000	-1.268970000000
O8	-0.545152000000	1.076749000000	1.379219000000
O9	-0.545212000000	1.076720000000	-1.379280000000
O10	1.770219000000	0.480562000000	0.000013000000
O11	-1.789778000000	-0.899352000000	-2.613747000000
O12	-1.789485000000	-0.899292000000	2.613284000000
O13	2.593544000000	-2.028134000000	0.000000000000
O14	0.815442000000	3.184071000000	0.000000000000
H15	-1.989564000000	-1.831092000000	-2.695214000000

V₂P₂O₁₀

PBE/LACVP** Energy: -1577.063965 Ha

M06/LACVP** Energy: -1577.671371 Ha

B3LYP/LACVP** Energy: -1578.055239 Ha

B3LYP/LACV3P** Energy: -1578.355090 Ha

B3LYP/mod-LACVP** Energy: -1578.027664 Ha

P1	3.783167000000	3.265940000000	2.419426000000
P2	1.390897000000	3.725535000000	3.854133000000
V3	2.995619000000	1.357612000000	4.502970000000
V4	1.474361000000	1.529740000000	1.911281000000
O5	1.799048000000	2.747810000000	5.179450000000
O6	4.476081000000	2.233488000000	3.573945000000
O7	2.749137000000	4.440543000000	3.104421000000
O8	2.024714000000	0.218022000000	3.249147000000
O9	3.057671000000	2.394037000000	1.157506000000
O10	0.380674000000	2.908315000000	2.762988000000
O11	4.932692000000	4.031683000000	1.795561000000
O12	3.684454000000	0.279570000000	5.996814000000
O13	0.569067000000	4.869992000000	4.412509000000
O14	0.448938000000	0.645634000000	0.484708000000

V₂P₂O₁₀H (POH)

PBE/LACVP** Energy: -1577.666094 Ha

M06/LACVP** Energy: -1578.291449 Ha
 B3LYP/LACVP** Energy: -1578.689930 Ha
 B3LYP/LACV3P** Energy: -1578.995134 Ha
 B3LYP/mod-LACVP** Energy: -1578.660813 Ha
 P1 -1.4777960000000 -0.0000540000000 1.1958000000000
 P2 1.4779450000000 0.0000430000000 1.1957180000000
 V3 0.0000360000000 1.4869270000000 -0.9509720000000
 V4 -0.0000130000000 -1.4869730000000 -0.9509290000000
 O5 1.3739020000000 1.2683180000000 0.1767090000000
 O6 -1.3741220000000 1.2684270000000 0.1769030000000
 O7 -0.0000070000000 0.0000080000000 1.9083060000000
 O8 0.0000030000000 0.0000130000000 -1.9342490000000
 O9 -1.3739940000000 -1.2682940000000 0.1767740000000
 O10 1.3739860000000 -1.2684240000000 0.1767500000000
 O11 -2.6005130000000 0.0000110000000 2.1368990000000
 O12 0.0000000000000 2.8266950000000 -1.7664190000000
 O13 2.6000660000000 0.0000000000000 2.1366130000000
 O14 0.0000000000000 -2.8266950000000 -1.7664190000000
 H15 -3.0462010000000 0.8283370000000 2.0527390000000

V₃PO₁₀

PBE/LACVP** Energy: -1307.316991 Ha
 M06/LACVP** Energy: -1307.716879 Ha
 B3LYP/LACVP** Energy: -1308.103335 Ha
 B3LYP/LACV3P** Energy: -1308.388222 Ha
 B3LYP/mod-LACVP** Energy: -1308.058472 Ha
 P1 3.8421970000000 3.2668990000000 2.3866310000000
 V2 1.3084280000000 3.8011950000000 3.9077410000000
 V3 3.0181070000000 1.3234340000000 4.5227740000000
 V4 1.4669730000000 1.5012980000000 1.8764860000000
 O5 1.8354620000000 2.6258600000000 5.3824920000000
 O6 4.4841110000000 2.2483610000000 3.5898670000000
 O7 2.9045640000000 4.5376210000000 3.0217260000000
 O8 2.0010140000000 0.2241800000000 3.2613420000000
 O9 3.0509560000000 2.4128150000000 1.1449720000000
 O10 0.2156630000000 2.8115400000000 2.6191290000000
 O11 5.0374480000000 3.9287690000000 1.7305130000000
 O12 3.7857880000000 0.1546400000000 5.9060160000000
 O13 0.2436770000000 5.2881120000000 4.6317330000000
 O14 0.5721310000000 0.5231970000000 0.4234370000000

V₃PO₁₀H

PBE/LACVP** Energy: -1307.930935 Ha
 M06/LACVP** Energy: -1308.342288 Ha
 B3LYP/LACVP** Energy: -1308.741312 Ha
 B3LYP/LACV3P** Energy: -1309.030320 Ha

B3LYP/mod-LACVP** Energy: -1308.694284 Ha

P1	3.8832020000000	3.2887890000000	2.3654880000000
V2	1.3078140000000	3.7641820000000	3.9043560000000
V3	2.9854430000000	1.3343670000000	4.5072530000000
V4	1.4631710000000	1.5085770000000	1.9133560000000
O5	1.9064190000000	2.6124900000000	5.1294300000000
O6	4.2209190000000	2.2421590000000	3.5773880000000
O7	2.8024260000000	4.2951300000000	3.0702800000000
O8	2.0533120000000	0.4804300000000	3.2474570000000
O9	2.9327330000000	2.3872730000000	1.3851780000000
O10	0.4679020000000	2.7799720000000	2.6746900000000
O11	5.0359910000000	3.9307460000000	1.7264920000000
O12	3.5713660000000	0.3926720000000	5.6195860000000
O13	0.4430220000000	4.9349010000000	4.4959490000000
O14	0.7343580000000	0.7161720000000	0.7690940000000
H15	5.2274170000000	4.8901200000000	1.6881070000000

V₄O₁₀

PBE/LACVP** Energy: -1037.560270 Ha

M06/LACVP** Energy: -1037.755956 Ha

B3LYP/LACVP** Energy: -1038.145038 Ha

B3LYP/LACV3P** Energy: -1038.414540 Ha

B3LYP/mod-LACVP** Energy: -1038.081099 Ha

V1	3.8861244000	3.2858457349	2.3643273784
V2	1.3026244892	3.7876619713	3.9099492482
V3	2.9987536401	1.3257209640	4.5214177189
V4	1.4605309250	1.5034371331	1.8936447668
O5	1.9247213885	2.6243922515	5.1169256389
O6	4.3352047017	2.1580394500	3.6761221131
O7	2.7521910590	4.4527801447	3.1055954634
O8	2.0719223250	0.4977925810	3.2374217963
O9	2.8989982039	2.3244924140	1.2271128670
O10	0.4915248383	2.7923927799	2.6666607041
O11	5.1240655368	3.9714620541	1.6805217183
O12	3.4861713690	0.3503763463	5.6539217076
O13	0.3679564026	4.8871945741	4.5353578194
O14	0.6620606799	0.6838385322	0.8167205101

V₄O₁₀H

PBE/LACVP** Energy: -1038.172814 Ha

M06/LACVP** Energy: -1038.369306 Ha

B3LYP/LACVP** Energy: -1038.769279 Ha

B3LYP/LACV3P** Energy: -1039.042990 Ha

B3LYP/mod-LACVP** Energy: -1038.705441 Ha

V1	3.8808750000000	3.2842520000000	2.3658030000000
V2	1.3065910000000	3.7812250000000	3.9083350000000

V3	2.9964140000000	1.3261690000000	4.5187430000000
V4	1.4632000000000	1.5044770000000	1.8937150000000
O5	1.9242270000000	2.6226170000000	5.1209550000000
O6	4.3340720000000	2.1620910000000	3.6800060000000
O7	2.7530380000000	4.4573450000000	3.1021700000000
O8	2.0709790000000	0.4926820000000	3.2374470000000
O9	2.9000000000000	2.3274540000000	1.2207630000000
O10	0.4868650000000	2.7898130000000	2.6656090000000
O11	5.1297270000000	3.9743260000000	1.6836150000000
O12	3.4922260000000	0.3486230000000	5.6527030000000
O13	0.3695820000000	4.8898850000000	4.5265200000000
O14	0.6537720000000	0.6863670000000	0.8183910000000
H15	4.7467270000000	4.7523040000000	2.0609080000000

VP₃O₁₀H (V=O)

PBE/LACVP** Energy: -1847.393225 Ha

M06/LACVP** Energy: -1848.224957 Ha

B3LYP/LACVP** Energy: -1848.622730 Ha

B3LYP/LACV3P** Energy: -1848.942884 Ha

B3LYP/mod-LACVP** Energy: -1848.612484 Ha

P1	-1.4770910064257	-0.0000095215325	1.1952928685957
P2	1.4772677470333	0.0001216723840	1.1952081771798
V3	0.0000368013232	1.4856119157088	-0.9500194425576
V4	0.0000067694990	-1.4856618247758	-0.9500239328195
O5	1.3742409601880	1.2687321288316	0.1767926272745
O6	-1.3744576470125	1.2688364312482	0.1769625387397
O7	-0.0000128622451	-0.0000193927601	1.9083698978343
O8	-0.0000050826666	-0.0000202980238	-1.9347076560941
O9	-1.3743392656431	-1.2687618233413	0.1768299142816
O10	1.3743072324036	-1.2688853484646	0.1768095327856
O11	-2.6008712130152	-0.0000890213538	2.1372043722560
O12	0.0000029860420	2.8274408294610	-1.7671507854626
O13	2.6004220070054	0.0000332067717	2.1369299680754
O14	-0.0000198519929	-2.8274294194886	-1.7670239496603
H15	-1.6494398974779	-2.1008941998828	0.5240953458284

V₂P₂O₁₀H (V-OH-P)

PBE/LACVP** Energy: -1577.642408 Ha

M06/LACVP** Energy: -1578.265815 Ha

B3LYP/LACVP** Energy: -1578.666723 Ha

B3LYP/LACV3P** Energy: -1578.973805 Ha

B3LYP/mod-LACVP** Energy: -1578.636850 Ha

P1	-0.9957000000000	-0.4843320000000	-1.4605270000000
P2	1.4545040000000	-1.1149560000000	-0.0000010000000
P3	-0.9956540000000	-0.4840840000000	1.4605430000000

V4	0.4300630000000	1.6651900000000	-0.0000350000000
O5	0.4299580000000	-1.2682660000000	1.2689990000000
O6	-1.6990910000000	-0.7206550000000	-0.0000010000000
O7	0.4299420000000	-1.2682450000000	-1.2689700000000
O8	-0.5451520000000	1.0767490000000	1.3792190000000
O9	-0.5452120000000	1.0767200000000	-1.3792800000000
O10	1.7702190000000	0.4805620000000	0.0000130000000
O11	-1.7897780000000	-0.8993520000000	-2.6137470000000
O12	-1.7894850000000	-0.8992920000000	2.6132840000000
O13	2.5935440000000	-2.0281340000000	0.0000000000000
O14	0.8154420000000	3.1840710000000	0.0000000000000
H15	1.3345686943251	3.3829819149717	-0.7826505753810

3.2 Optimized VPO Slabs

(VO)₂P₂O₇

Energy: -6162.931036 Ha

a = 8.36200000

b = 9.53603000

V	3.073521623314E-01	1.449295745816E-02	8.140053985460E+00
V	1.863320061084E-01	-4.967996728959E-01	1.188605449705E+01
V	-3.093082399117E-01	1.455517370300E-02	1.262497676842E+01
V	-1.882157539541E-01	-4.968077053428E-01	8.878848445264E+00
V	-3.137265377222E-01	3.197689014441E-03	8.879361619588E+00
V	-1.925434851149E-01	-4.854792604723E-01	1.262544920603E+01
V	3.118262259716E-01	3.188505230633E-03	1.188581694705E+01
V	1.906794507511E-01	-4.854831118992E-01	8.139596028166E+00
P	-8.077151234361E-03	2.085369321692E-01	8.103200888771E+00
P	-4.992450234770E-01	3.086914132896E-01	1.196530873217E+01
P	6.180623186656E-03	2.085180055952E-01	1.266202069736E+01
P	4.973271113545E-01	3.086637907415E-01	8.798680939820E+00
P	7.304006694511E-04	-1.913423707378E-01	8.799660358217E+00
P	4.919912954994E-01	-2.914654952495E-01	1.266220708507E+01
P	-2.625463648522E-03	-1.913223723279E-01	1.196664638387E+01
P	-4.938634791033E-01	-2.914605767994E-01	8.101989076618E+00
O	-3.029472022990E-01	5.318447607772E-02	1.416965593645E+01
O	-1.687612846301E-01	1.582668952273E-01	8.690307226253E+00
O	-1.406579725670E-01	1.426359127557E-01	1.197822185326E+01
O	-4.971632098088E-01	1.427010943697E-01	8.655452046188E+00
O	-1.805660971743E-01	4.700479889703E-01	1.043080781766E+01
O	-3.427716464133E-01	3.583871615363E-01	1.258188381693E+01
O	-3.547163721494E-01	3.802919014374E-01	8.202903452279E+00
O	5.310530582639E-03	3.769074059039E-01	1.254140306868E+01
O	3.009570433490E-01	5.311390057984E-02	6.595324409403E+00
O	1.668711311044E-01	1.582445361975E-01	1.207516231793E+01
O	1.387690119696E-01	1.426447917428E-01	8.786854945333E+00

O	4.952855371269E-01	1.427211990472E-01	1.210884029359E+01
O	1.785776915856E-01	4.699867897273E-01	1.033415584464E+01
O	3.409057319294E-01	3.583732232519E-01	8.181097668313E+00
O	3.528483475210E-01	3.803227382608E-01	1.256215751764E+01
O	-7.182802991270E-03	3.769264660085E-01	8.224067756626E+00
O	3.194988149587E-01	-3.007199141021E-02	1.033408436976E+01
O	1.572181889982E-01	-1.416013030823E-01	8.182823415200E+00
O	1.453381001718E-01	-1.196933458772E-01	1.256223441237E+01
O	-4.947163565377E-01	-1.230894697118E-01	8.223524834468E+00
O	1.970263024491E-01	-4.468779836770E-01	6.594937594165E+00
O	3.313340834394E-01	-3.417326036157E-01	1.207449700050E+01
O	3.593243366454E-01	-3.573870990757E-01	8.785963771212E+00
O	2.856660585315E-03	-3.572930429654E-01	1.211071232975E+01
O	-3.214314006897E-01	-3.003332678508E-02	1.043118562441E+01
O	-1.590446057561E-01	-1.415725027592E-01	1.258379039079E+01
O	-1.471631587332E-01	-1.196547215980E-01	8.203389370341E+00
O	4.928472898508E-01	-1.230829571281E-01	1.254134063461E+01
O	-1.991283776309E-01	-4.470361994457E-01	1.417040132110E+01
O	-3.331516416644E-01	-3.417430869412E-01	8.688509073127E+00
O	-3.611331225389E-01	-3.573421285645E-01	1.197888902560E+01
O	-4.726834122776E-03	-3.572854345419E-01	8.655299512210E+00
O	3.061476715165E-03	1.746369906297E-01	1.422155700975E+01
O	-5.004448344976E-03	1.746935271792E-01	6.543470404631E+00
O	4.988890895497E-01	3.421917057317E-01	1.038201684799E+01
O	-9.811317716647E-04	-1.579234793732E-01	1.038305563263E+01
O	4.949899613077E-01	-3.253317123765E-01	1.422198601925E+01
O	-4.969758713492E-01	-3.252579635693E-01	6.542068231753E+00
H	-4.018645620290E-01	-3.642632551211E-01	1.450296006149E+01
H	3.998326219407E-01	-3.641105485156E-01	6.261399558980E+00
H	-1.001832678619E-01	1.358628036283E-01	1.450200072259E+01
H	9.820000257647E-02	1.358688103947E-01	6.262735201197E+00

(VO)₂P₂O₇H (VOH)

Energy: -6163.549609 Ha

a = 8.36200000

b = 9.53603000

V	3.068360054856E-01	1.511207469781E-02	8.150882128139E+00
V	1.871581674120E-01	-4.960123872048E-01	1.191545774597E+01
V	-3.097549830194E-01	1.498858074562E-02	1.263714199766E+01
V	-1.886793281326E-01	-4.954112470127E-01	8.875777187038E+00
V	-3.140329825963E-01	4.437093899759E-03	8.883360469977E+00
V	-1.949767856747E-01	-4.856959345554E-01	1.247816765177E+01
V	3.115430488327E-01	2.620311518974E-03	1.189635818132E+01
V	1.905628664502E-01	-4.843167800014E-01	8.159525729560E+00
P	-8.210630366593E-03	2.098260937303E-01	8.113774826000E+00

P -4.996172509499E-01 3.079920699417E-01 1.195816140718E+01
P 8.354239220032E-03 2.092142114336E-01 1.271640972024E+01
P 4.968551799561E-01 3.095040570867E-01 8.795549965216E+00
P -2.131772075219E-04 -1.898410059618E-01 8.800800842928E+00
P 4.909161811793E-01 -2.896874183536E-01 1.272755985510E+01
P -4.384679290154E-03 -1.904162102891E-01 1.196092726305E+01
P -4.942834634125E-01 -2.902653266679E-01 8.097883770230E+00
O -3.024370048426E-01 5.293981132625E-02 1.418433957459E+01
O -1.689480528196E-01 1.596052282677E-01 8.697139572021E+00
O -1.370834958333E-01 1.423956367554E-01 1.201688358233E+01
O -4.972461222267E-01 1.437056847198E-01 8.647683454471E+00
O -1.810569021474E-01 4.720470759515E-01 1.043988962970E+01
O -3.412377227452E-01 3.567180624168E-01 1.254898471464E+01
O -3.544611999202E-01 3.813579465835E-01 8.208619387309E+00
O 1.082634482910E-02 3.770134797915E-01 1.260807196086E+01
O 2.999498573811E-01 5.384613325501E-02 6.606074909339E+00
O 1.697065729716E-01 1.576905060341E-01 1.215071970421E+01
O 1.386136022463E-01 1.440355925913E-01 8.797002232270E+00
O 4.956089178927E-01 1.423037655099E-01 1.210322453939E+01
O 1.806748332958E-01 4.728352141496E-01 1.035393696129E+01
O 3.409595013849E-01 3.596661828515E-01 8.171529532078E+00
O 3.544236643997E-01 3.803113605024E-01 1.257044632663E+01
O -7.615475337019E-03 3.784588484715E-01 8.239219023586E+00
O 3.183838281516E-01 -2.942407460104E-02 1.033808221622E+01
O 1.565939966256E-01 -1.410291868043E-01 8.182566023411E+00
O 1.420128951993E-01 -1.178916796580E-01 1.256627425340E+01
O -4.947273486904E-01 -1.221709170188E-01 8.227916631503E+00
O 1.956187087774E-01 -4.447527805854E-01 6.616160412771E+00
O 3.248088237485E-01 -3.404479512911E-01 1.223752521380E+01
O 3.603541571654E-01 -3.565403855683E-01 8.797638173254E+00
O 2.055381992032E-03 -3.563095100810E-01 1.208430407653E+01
O -3.215080050284E-01 -2.818319150190E-02 1.043598319826E+01
O -1.618155847245E-01 -1.422724407714E-01 1.257424676171E+01
O -1.477475831414E-01 -1.181502532897E-01 8.197610153282E+00
O 4.896712381205E-01 -1.204799116834E-01 1.257580549672E+01
O -2.090817988309E-01 -4.373809305120E-01 1.424339514777E+01
O -3.320584567570E-01 -3.410863913579E-01 8.658110042942E+00
O -3.706399318118E-01 -3.547714202831E-01 1.194335222381E+01
O -5.880614532827E-03 -3.560921855634E-01 8.664507756888E+00
O -3.242105194924E-04 1.771629574465E-01 1.428323215194E+01
O -4.677932311681E-03 1.769173032379E-01 6.552625630253E+00
O 4.971121604919E-01 3.423272161686E-01 1.037565099701E+01
O -2.387942911831E-03 -1.552678777520E-01 1.037823195254E+01
O -4.914082991070E-01 -3.201233910691E-01 1.427604359413E+01
O -4.996615868167E-01 -3.233920469683E-01 6.537755891703E+00
H -3.842669390849E-01 -3.628250834157E-01 1.447318678787E+01

H	3.966404938798E-01	-3.620451786068E-01	6.266575250043E+00
H	-1.009840499857E-01	1.303148597470E-01	1.451685267419E+01
H	9.839491269773E-02	1.375520415954E-01	6.274065494112E+00
H	-1.350450140105E-01	-4.752166209980E-01	1.489379794784E+01

(VO)₂P₂O₇H (V-OH-P)

Energy: -6163.478075 Ha

a = 8.36200000

b = 9.53603000

V	3.068527869466E-01	1.755636998125E-02	8.131634848975E+00
V	1.774202348013E-01	-4.901806900916E-01	1.193736233247E+01
V	-3.056978304536E-01	9.658132623333E-03	1.262849513985E+01
V	-1.891939785321E-01	-4.938023982369E-01	8.837883672259E+00
V	-3.143305471597E-01	3.204427405806E-03	8.890529508756E+00
V	-1.997150483633E-01	-4.861206918694E-01	1.236220777636E+01
V	3.107792984024E-01	-1.280708719641E-03	1.188873169231E+01
V	1.880978010757E-01	-4.815679343820E-01	8.154675169305E+00
P	-8.789906555349E-03	2.098091668314E-01	8.139279076871E+00
P	-4.900871921223E-01	2.988851616970E-01	1.195230031588E+01
P	1.101737249959E-02	2.083528736956E-01	1.262767505410E+01
P	4.897205050913E-01	3.075473273304E-01	8.817973227640E+00
P	3.872437617380E-03	-1.864709384763E-01	8.795794238823E+00
P	4.909833361076E-01	-2.919929022035E-01	1.280314546751E+01
P	-2.755623350757E-03	-1.873320334740E-01	1.191071158658E+01
P	-4.966141835499E-01	-2.868178324974E-01	8.000341829017E+00
O	-2.973453084157E-01	5.192223712951E-02	1.416470480345E+01
O	-1.714849557490E-01	1.592332954561E-01	8.697691975928E+00
O	-1.369751984446E-01	1.404530762741E-01	1.197783133849E+01
O	4.962043330768E-01	1.419404003871E-01	8.758218441491E+00
O	-1.875948074833E-01	4.739911628662E-01	1.055147956276E+01
O	-3.471666988137E-01	3.542717359810E-01	1.269402543610E+01
O	-3.635357480801E-01	3.767434080431E-01	8.262466050703E+00
O	9.627500623133E-03	3.758779498676E-01	1.252291607767E+01
O	3.029996134427E-01	6.390818617754E-02	6.606317326129E+00
O	1.731915184201E-01	1.608054829686E-01	1.202803023772E+01
O	1.355962430203E-01	1.403696621761E-01	8.831375344590E+00
O	4.963460663537E-01	1.370799402204E-01	1.211604633194E+01
O	1.955215241725E-01	4.772228549383E-01	1.039883115950E+01
O	3.317507359208E-01	3.570644260049E-01	8.241876356813E+00
O	3.581186087063E-01	3.755724904393E-01	1.274510168235E+01
O	-5.327388515854E-03	3.776360160249E-01	8.281281104244E+00
O	3.207340347854E-01	-4.033650993841E-02	1.035397113598E+01
O	1.580212161128E-01	-1.369234215555E-01	8.131192564047E+00
O	1.399093165670E-01	-1.147705195774E-01	1.258578796657E+01
O	-4.953586455586E-01	-1.182148625572E-01	8.188775047477E+00

O	1.896970133461E-01	-4.468263486437E-01	6.601958028458E+00
O	3.188945985643E-01	-3.479976853110E-01	1.255984636577E+01
O	3.607189327309E-01	-3.542818394003E-01	8.738413827021E+00
O	6.009725317617E-03	-3.518936071023E-01	1.195021408993E+01
O	-3.237621915951E-01	-3.148386192226E-02	1.044497549468E+01
O	-1.628945685276E-01	-1.471147865561E-01	1.253987663739E+01
O	-1.462507119051E-01	-1.173375294482E-01	8.207587723200E+00
O	4.879575938769E-01	-1.244048561991E-01	1.263688069633E+01
O	-1.894101982789E-01	-4.339596126634E-01	1.392060259123E+01
O	-3.328007354699E-01	-3.388859562728E-01	8.466893089185E+00
O	-3.853874204444E-01	-3.607542333076E-01	1.188631833749E+01
O	4.159865575409E-03	-3.510478279971E-01	8.761302874777E+00
O	1.268179920085E-02	1.722608282987E-01	1.418639885476E+01
O	-5.140975071078E-03	1.776633992648E-01	6.576236059516E+00
O	4.827880365643E-01	3.427975424224E-01	1.046991923877E+01
O	2.902065229228E-03	-1.409354826496E-01	1.036682570077E+01
O	-4.698344468848E-01	-3.260022086591E-01	1.432476499357E+01
O	4.848125072723E-01	-3.110277836157E-01	6.431995608049E+00
H	-3.560325456083E-01	-3.591410583493E-01	1.440399442865E+01
H	3.810507222809E-01	-3.524328458638E-01	6.205130772751E+00
H	-9.026798682552E-02	1.348242728251E-01	1.448527817459E+01
H	9.939822145183E-02	1.424666176116E-01	6.286706369823E+00
H	4.048192766048E-01	4.224205225984E-01	1.352261916263E+01

α_1 -VOPO₄

Energy: -1577.652242 Ha

a = 6.14123848

b = 6.14323930

O	-4.561940696074E-01	-3.027157513083E-01	1.079454573575E+00
P	-4.830539238612E-01	4.938396249476E-01	2.002492567549E+00
O	4.900912504574E-01	2.903875577379E-01	1.079462804099E+00
O	-1.865415547869E-01	2.067301714995E-02	1.078145071316E+00
O	2.204363925968E-01	-3.301183362953E-02	1.078131781766E+00
O	-9.910151581224E-03	-2.096149110898E-01	2.924666620626E+00
O	4.380595827446E-02	1.972809027336E-01	2.924657450453E+00
O	-2.795650413035E-01	4.669925968506E-01	2.925983104903E+00
O	3.134564849969E-01	-4.793234412240E-01	2.925955485346E+00
V	1.694278120000E-02	4.938333875068E-01	2.469951139144E+00
O	1.693768456465E-02	4.938312339038E-01	9.159440695867E-01
V	-4.830509021492E-01	-6.157301981876E-03	1.534163741988E+00
O	-4.830453455772E-01	-6.153656128312E-03	3.088168569596E+00
P	1.695024477649E-02	-6.167573468704E-03	2.001623020055E+00

α_1 -VOPO₄H (VOH)

Energy: -1578.263588 Ha

a = 6.14123848

b = 6.14323930

O -4.491755899455E-01 -3.017554733509E-01 1.125538239769E+00
P -4.921760149192E-01 4.974250058641E-01 2.012499174960E+00
O 4.722562733742E-01 2.986998758136E-01 1.073517085699E+00
O -1.874294495914E-01 3.033120733602E-02 1.012903600417E+00
O 2.156987543853E-01 -4.125667126048E-02 1.077106638819E+00
O -3.013356799051E-02 -2.119327049087E-01 2.872478921507E+00
O 3.646296222249E-02 1.933264294011E-01 2.915069902635E+00
O -2.921672234159E-01 4.525008052169E-01 2.958456430934E+00
O 3.019780028596E-01 -4.730787809151E-01 2.930102310962E+00
V 7.876554640659E-03 4.920960054669E-01 2.466632182369E+00
O 7.578843468103E-03 4.893251724444E-01 9.140651669817E-01
V -4.839609976968E-01 1.147237808244E-03 1.414925884122E+00
O -4.717301727652E-01 9.790412861257E-03 3.161087897711E+00
P 1.120699360744E-02 -7.894740613816E-03 1.960995374612E+00
H -3.920709058104E-01 1.322600708363E-01 3.555401188501E+00

α_1 -VOPO₄H (V-OH-P)

Energy: -1578.266830 Ha

a = 6.14123848

b = 6.14323930

O -4.262855964489E-01 -2.924511449337E-01 1.169811443918E+00
P -4.953693643849E-01 -4.924034343864E-01 1.984066447266E+00
O 4.850932029584E-01 3.046869661633E-01 1.071413037092E+00
O -1.822898288844E-01 4.144831812654E-02 1.117498628248E+00
O 2.303015397643E-01 -3.465374318537E-02 1.197021352758E+00
O -2.882564920948E-02 -2.016365210911E-01 2.948924586280E+00
O 4.817824316809E-02 2.014281634135E-01 3.003982418201E+00
O -2.914679046886E-01 4.563058674438E-01 3.022419479679E+00
O 3.177798149671E-01 -4.548079084041E-01 2.950617306504E+00
V 2.118544688949E-02 -4.986477688796E-01 2.379719376124E+00
O 1.875933848187E-02 4.959596195036E-01 8.102443086184E-01
V -4.750870690307E-01 9.459553389965E-03 1.563060648169E+00
O -4.691026637370E-01 2.481991457672E-02 3.125894146272E+00
P 1.934103579316E-02 4.985334217737E-04 2.095324637185E+00
H -3.145157789421E-01 3.206800336901E-01 3.514785288586E+00

α_2 -VOPO₄

Energy: -1577.646827 Ha

a = 5.96830081

b = 5.96815808

O 1.799995897769E-01 -4.969133375865E-02 2.202449811905E+00
O 3.200015199869E-01 -4.503087721803E-01 2.202454322514E+00
O -4.503050563317E-01 1.799972044354E-01 2.202337459331E+00
O -4.969337625938E-02 3.200039590122E-01 2.202351078951E+00

O -1.799993760280E-01 4.969147146735E-02 4.017445428783E+00
 O -3.200016535566E-01 4.503082904028E-01 4.017444207508E+00
 O 4.503048039036E-01 -1.799965345564E-01 4.017557031119E+00
 O 4.969384013311E-02 -3.200034492880E-01 4.017547863851E+00
 V 2.500006502321E-01 2.499995104533E-01 1.793003188729E+00
 O 2.499985158529E-01 2.500003954314E-01 2.366900688842E-01
 V -2.500005863999E-01 -2.500001508940E-01 4.426886611855E+00
 O -2.499990801151E-01 -2.500003461660E-01 5.983198027113E+00
 P 2.499998793991E-01 -2.500003260959E-01 3.110014903803E+00
 P -2.499996715938E-01 2.500000807368E-01 3.109879995654E+00

α_2 -VOPO₄H (VOH)

Energy: -1578.263222 Ha

a = 5.96830081

b = 5.96815808

O 1.771306923288E-01 -5.012674287575E-02 2.156797702899E+00
 O 3.162126537476E-01 -4.502772059879E-01 2.150477748479E+00
 O -4.532857623707E-01 1.807536321315E-01 2.181629474464E+00
 O -5.393753260047E-02 3.197004345820E-01 2.177262507324E+00
 O -1.798807992538E-01 4.889019642402E-02 3.994955338189E+00
 O -3.251479244157E-01 4.490601687868E-01 4.015475395668E+00
 O 4.481189222403E-01 -1.774712892104E-01 3.960504390101E+00
 O 4.674860306228E-02 -3.242737075598E-01 3.966974701180E+00
 V 2.464235747365E-01 2.496501734347E-01 1.756739941015E+00
 O 2.466079850347E-01 2.492858455280E-01 2.005529770832E-01
 V -2.524852959197E-01 -2.504643103415E-01 4.430764984520E+00
 O -2.504757741642E-01 -2.407463213229E-01 6.167746450520E+00
 P 2.470694736222E-01 -2.505700653793E-01 3.068690140111E+00
 P -2.533734145110E-01 2.502795263907E-01 3.089889081969E+00
 H -2.097244925465E-01 -9.574553560002E-02 6.537789166478E+00

α_2 -VOPO₄H (V-OH-P)

Energy: -1578.259508 Ha

a = 5.96830081

b = 5.96815808

O 1.579432638509E-01 -5.346762230345E-02 2.194631909180E+00
 O 3.160356956930E-01 -4.436016507628E-01 2.151782131184E+00
 O -4.629270178764E-01 1.824749482632E-01 2.181009873701E+00
 O -5.740597744191E-02 3.228695883708E-01 2.172328769371E+00
 O -1.777214529225E-01 5.343375962421E-02 3.965990880602E+00
 O -3.351568702861E-01 4.533510096090E-01 3.962090987106E+00
 O 4.359244002863E-01 -1.604624779336E-01 4.027182972446E+00
 O 6.632011582979E-02 -3.351936023463E-01 4.126485184640E+00
 V 2.394545091294E-01 2.517068884632E-01 1.774799037837E+00
 O 2.398297567665E-01 2.480219484006E-01 2.195573090392E-01
 V -2.632712897009E-01 -2.442196348717E-01 4.530069617311E+00

O -2.488398329308E-01 -2.509772791239E-01 6.104223976991E+00
P 2.587725949181E-01 -2.422262623311E-01 3.045958903104E+00
P -2.594430387596E-01 2.522400094390E-01 3.113497682319E+00
H 1.401789851908E-01 -3.539530447600E-01 4.987190765169E+00

X1-VOPO₄

Energy: -3155.167717 Ha

a = 9.36194256

b = 7.73512494

V 8.529480457934E-03 2.906429092191E-01 3.226104514598E+00
P 2.187346594007E-01 -1.133962645548E-02 3.870274051895E+00
O 1.453907655255E-01 -1.916714324142E-01 3.546374258264E+00
O 1.317969941757E-01 4.791404868536E-01 2.761689970545E+00
O -4.850089099372E-01 -2.218780765275E-01 1.097809590363E+00
O 3.727762751848E-01 -3.776677783798E-01 2.987389539302E+00
O -1.260581219464E-02 2.758813607953E-01 4.763874706429E+00
O 1.332220472102E-01 1.216392778561E-01 2.892045802221E+00
V 4.968031150964E-01 -2.086539412966E-01 2.639897618477E+00
P 2.877238783617E-01 4.872020001331E-01 2.024494762751E+00
O 3.609374048266E-01 3.079310515757E-01 2.377489500222E+00
O 3.746568271927E-01 -2.082707576153E-02 3.133712875971E+00
V -1.767335433691E-03 -2.892685072221E-01 2.656030400652E+00
P -2.120871296269E-01 1.257128791591E-02 2.013133915585E+00
O -1.388723878629E-01 1.928289846376E-01 2.340858612773E+00
O -1.251824121978E-01 -4.778813950434E-01 3.115994754889E+00
O 4.915454385640E-01 2.234063675079E-01 4.781019481346E+00
O -3.662330299242E-01 3.788799214580E-01 2.890103618295E+00
O 1.980678562506E-02 -2.737554295958E-01 1.119192607937E+00
O -1.267145953238E-01 -1.205633520563E-01 2.991028484323E+00
V -4.902706381557E-01 2.099446697842E-01 3.239166265360E+00
P -2.811099679066E-01 -4.860211339614E-01 3.853048209840E+00
O -3.544298661001E-01 -3.067940564274E-01 3.500738670457E+00
O -3.681586961361E-01 2.199226104930E-02 2.747201032891E+00
O 2.251171283526E-01 3.994192222360E-02 5.283053051977E+00
O -2.750492644782E-01 4.661361396114E-01 5.273180293624E+00
O 2.817117714208E-01 -4.650440087381E-01 6.042085868184E-01
O -2.182376221171E-01 -3.845159974106E-02 5.996748221943E-01

X1-VOPO₄H (VOH)

Energy: -3155.815461 Ha

a = 9.36194256

b = 7.73512494

V 2.108046281478E-02 3.177756074483E-01 3.580538134095E+00
P 2.134841118530E-01 -4.198395141246E-02 3.546230028118E+00
O 1.455972405325E-01 -1.480318206476E-01 2.302073795835E+00
O 1.353322525179E-01 4.958539815658E-01 2.654964965891E+00

O -4.429285790575E-01 -2.334755213898E-01 1.272074971200E+00
 O 3.783148263926E-01 -3.693253054663E-01 2.973918200343E+00
 O 3.809348958564E-03 3.576125661390E-01 5.208041289846E+00
 O 1.599191951873E-01 1.482369574680E-01 3.399991310808E+00
 V -4.853335878553E-01 -2.087414734625E-01 2.762141606328E+00
 P 2.933015804707E-01 -4.971543907899E-01 1.950665205329E+00
 O 3.669016744389E-01 3.192200690602E-01 2.225674297902E+00
 O 3.820697280435E-01 -1.939525194533E-02 3.019930504478E+00
 V -3.707082305105E-03 -2.964407588302E-01 2.270600595635E+00
 P -2.039624317805E-01 2.992125072945E-02 2.278666840156E+00
 O -1.269611640810E-01 1.769393196728E-01 3.087267777958E+00
 O -1.221793119630E-01 -4.822527304810E-01 3.117174603119E+00
 O 4.599635190137E-01 2.338691682244E-01 4.734669708374E+00
 O -3.666279211300E-01 3.740433055216E-01 2.977249511555E+00
 O -3.344948545973E-02 -3.167542108401E-01 7.539320000718E-01
 O -1.317595086460E-01 -1.432797134812E-01 2.880862705784E+00
 V 4.970320592018E-01 2.081946537586E-01 3.229938716793E+00
 P -2.737594913398E-01 -4.973198238582E-01 3.871342438151E+00
 O -3.535793064893E-01 -3.185383637764E-01 3.815892120004E+00
 O -3.645214647971E-01 1.999257587070E-02 2.985637841976E+00
 O 2.006787357710E-01 -1.315826314864E-01 4.842578466750E+00
 O -2.466846880823E-01 4.397563050964E-01 5.279016413814E+00
 O 2.900967887139E-01 -4.418651825600E-01 5.468671944345E-01
 O -2.092215712865E-01 4.395986278814E-02 8.135574449443E-01
 H -1.077986656370E-01 3.931213250838E-01 5.431391310309E+00

X1-VOPO₄H (V-O(1)H-P)

Energy: -3155.783526 Ha

a = 9.36194256

b = 7.73512494

V 3.160053626551E-02 3.164882880410E-01 3.517388480046E+0
 P 2.099037587221E-01 -4.169828205480E-02 3.369328433599E+0
 O 1.413961845842E-01 -1.616870204073E-01 2.225268947939E+0
 O 1.275255569395E-01 4.900167686995E-01 2.458284499649E+0
 O -4.372449747366E-01 -2.175147176448E-01 1.296352111428E+0
 O 3.708170527212E-01 -3.803704646567E-01 2.794110819328E+0
 O 7.131447718473E-02 3.503695839208E-01 5.000284560710E+0
 O 1.468298363354E-01 1.450583674209E-01 2.968546361532E+0
 V -4.949680996757E-01 -2.237532081839E-01 2.757436169364E+0
 P 2.874020600186E-01 4.969998134509E-01 1.676708600895E+0
 O 3.574786768884E-01 3.186138996461E-01 1.871254867331E+0
 O 3.780467840224E-01 -2.497908020547E-02 2.928700527372E+0
 V -1.139453841220E-02 -3.075445334049E-01 2.263902775935E+0
 P -1.955125027082E-01 3.565168446916E-02 2.630334930516E+0
 O -1.228561044131E-01 1.700684480565E-01 3.594858518930E+0
 O -1.190059786771E-01 -4.870094166291E-01 3.185826206987E+0

O 4.240295374398E-01 2.588762885215E-01 4.585117778169E+0
 O -3.658282206826E-01 3.784597701560E-01 2.831276204559E+0
 O -5.848628185061E-02 -3.164723221156E-01 7.792727489325E-1
 O -1.260660084547E-01 -1.426067693001E-01 3.032694382686E+0
 V 4.821395162887E-01 2.153050327629E-01 3.155347052165E+0
 P -2.826011961123E-01 4.898140429906E-01 3.876132554523E+0
 O -3.585089089604E-01 -3.205304007944E-01 3.778621700053E+0
 O -3.571495361961E-01 1.755802062202E-02 3.471627994047E+0
 O 1.862123610307E-01 -9.982923174160E-02 4.754418084563E+0
 O -2.673728702708E-01 4.295360730330E-01 5.267525624394E+0
 O 2.722917056883E-01 -4.230957827552E-01 3.532937109647E-1
 O -2.262473392266E-01 7.684400207121E-02 1.229245357087E+0
 H -3.388792820595E-01 -2.255390263685E-03 4.422789996296E+0

X1-VOPO₄H (V-O(2)H-P)

Energy: -3155.794270 Ha

a = 9.36194256

b = 7.73512494

V 1.059705175888E-02 2.911857226285E-01 3.285095147480E+00
 P 2.224544269788E-01 -9.590958676117E-03 3.858285438675E+00
 O 1.537498159701E-01 -1.970694837724E-01 3.535637016572E+00
 O 1.346271896016E-01 4.740446297021E-01 2.759006348235E+00
 O -4.716504112142E-01 -2.379445518300E-01 1.065686406467E+00
 O 3.696045807636E-01 -3.897807186944E-01 3.092573189244E+00
 O -4.502375246886E-03 2.751106324986E-01 4.827980743644E+00
 O 1.323917900788E-01 1.198048612399E-01 2.899681971236E+00
 V -4.858099790480E-01 -1.973997110023E-01 2.591246677271E+00
 P 2.877033736052E-01 4.812658500685E-01 1.980823275115E+00
 O 3.645271195010E-01 3.036942238844E-01 2.224463235217E+00
 O 3.759388049061E-01 -1.704679991984E-02 3.132683190698E+00
 V -4.264844419639E-03 -2.918775619055E-01 2.685678887862E+00
 P -2.058584945715E-01 1.694678397340E-02 2.019464806603E+00
 O -1.369942604308E-01 1.969766769800E-01 2.395385583173E+00
 O -1.208358233081E-01 -4.789781492887E-01 3.212113648096E+00
 O 4.833255151153E-01 2.309242812126E-01 4.729164232420E+00
 O -3.645129529614E-01 3.788959789009E-01 2.901661580689E+00
 O 1.103501792509E-02 -2.851548549414E-01 1.139392694535E+00
 O -1.216946365426E-01 -1.176800298254E-01 3.012950874318E+00
 V -4.897475282528E-01 2.116167947556E-01 3.202174637061E+00
 P -2.812395293255E-01 -4.892662788183E-01 3.943771681616E+00
 O -3.495577304667E-01 -3.108423195020E-01 3.681340672273E+00
 O -3.628824428375E-01 2.374353296112E-02 2.727121863761E+00
 O 2.241442468654E-01 3.625701362412E-02 5.285327831018E+00
 O -2.704127552539E-01 4.410351848584E-01 5.308496957325E+00
 O 2.809875368346E-01 -4.519870778498E-01 6.123704317115E-01
 O -2.061388290916E-01 -3.201918800129E-02 6.025251519104E-01

H 2.908171527113E-01 -3.342108905716E-01 3.604035825773E+00

X1-VOPO₄H (POH)

Energy: -3155.836117 Ha

a = 9.36194256

b = 7.73512494

V 1.734988905623E-01 2.428577764187E+00 3.546514510305E+00
P 1.970972787759E+00 -1.310849808803E-01 3.483540025468E+00
O 1.353289507860E+00 -1.524132144486E+00 3.221885508227E+00
O 1.211685728773E+00 3.756786950504E+00 2.506165878750E+00
O -4.225838635742E+00 -1.799490397734E+00 1.133613758663E+00
O 3.510067731093E+00 -2.916716245699E+00 2.854067937330E+00
O 7.379743209110E-01 2.486044215437E+00 5.028019863769E+00
O 1.217309728555E+00 9.886686603661E-01 2.779043518050E+00
V 4.761032842788E+00 -1.657953383048E+00 2.635992970092E+00
P 2.678549819325E+00 3.838887458309E+00 1.830125022577E+00
O 3.383657946010E+00 2.419438145192E+00 2.114708621031E+00
O 3.482141539460E+00 -1.766207269560E-01 2.957405608311E+00
V -1.163395159336E-01 -2.340412473520E+00 2.473632796770E+00
P -1.907411604069E+00 2.833683512303E-01 2.481960094973E+00
O -1.349237454694E+00 1.279202009844E+00 3.532931196227E+00
O -1.180704924557E+00 -3.787860052932E+00 3.181840099981E+00
O 4.265923140734E+00 1.843617694354E+00 4.619674510284E+00
O -3.448701695889E+00 2.870045118314E+00 2.862352787212E+00
O -1.266867998522E-01 -2.172079352028E+00 9.288917352276E-01
O -1.273061546626E+00 -1.134150471722E+00 3.022901629624E+00
V -4.714925632083E+00 1.633088701361E+00 3.121769904150E+00
P -2.657362987340E+00 -3.891865653790E+00 3.897421344737E+00
O -3.355091433335E+00 -2.482839707826E+00 3.641520389219E+00
O -3.503705203614E+00 1.192371356628E-01 2.920092021569E+00
O 2.044727612752E+00 5.994205666621E-02 5.047165698116E+00
O -2.596055864844E+00 3.412083838012E+00 5.299918784379E+00
O 2.691507665724E+00 -3.441949108806E+00 4.332004617762E-01
O -1.724924482895E+00 5.104281140083E-01 1.038713724231E+00
H 1.676138648081E+00 9.210682972958E-01 5.350539598951E+00

3.3 Optimized Intermediates – Gas Phase Species

Butane

Energy: -158.475970 Ha

C	0.4332800463	1.9144856519	0.0000000000
C	-0.4196017539	0.6421282967	0.0000000000
C	0.4192904552	-0.6419520775	0.0000000000
C	-0.4330324372	-1.9146459104	0.0000000000
H	-0.1877518384	2.8167534647	0.0000000000
H	1.0804035192	1.9540055133	0.8842193409

H	1.0804035192	1.9540055133	-0.8842193409
H	-1.0805803286	0.6412685853	-0.8780518996
H	-1.0805803286	0.6412685853	0.8780518996
H	1.0802845393	-0.6409403224	0.8780745663
H	1.0802845393	-0.6409403224	-0.8780745663
H	0.1885809835	-2.8165043238	0.0000000000
H	-1.0801431318	-1.9545533672	0.8842302595
H	-1.0801431318	-1.9545533672	-0.8842302595

Activated Butane

Energy: -157.56246 Ha

C	-8.4099587976	1.5400012914	2.2192486137
C	-7.1021272384	2.2215375602	1.9923128922
C	-5.8067964450	1.4925554861	2.1496706104
C	-4.5879248238	2.4214046453	2.2354102489
H	-9.2360497265	2.2540383804	2.3022128135
H	-8.6675714711	0.8484876067	1.3966694687
H	-8.3926963772	0.9313998420	3.1336239220
H	-7.0926283487	3.1733871817	1.4638048748
H	-5.6616346435	0.7895650575	1.3067415800
H	-5.8522397137	0.8513484807	3.0433066074
H	-3.6572522263	1.8532313018	2.3319470082
H	-4.5081008378	3.0440050905	1.3369879862
H	-4.6680647248	3.0924277934	3.0971437882

2-butene

Energy: -157.233275 Ha

C	0.5326457930	1.8972904721	0.0000000000
C	-0.2655463986	0.6123362152	0.0000000000
C	0.2655612055	-0.6123109810	0.0000000000
C	-0.5326636562	-1.8973075220	0.0000000000
H	-0.1197747143	2.7750883258	0.0000000000
H	1.1799527384	1.9709368354	0.8820027622
H	1.1799527384	1.9709368354	-0.8820027622
H	-1.3524959122	0.7086205212	0.0000000000
H	1.3525226383	-0.7086610760	0.0000000000
H	0.1197888632	-2.7751048965	0.0000000000
H	-1.1799549800	-1.9709569972	0.8820140777
H	-1.1799549800	-1.9709569972	-0.8820140777

Butenyl radical

Energy: -156.558844 Ha

C	0.6516325418	1.8105208198	0.0000000000
C	-0.2469989938	0.5942570837	0.0000000000
C	0.1908610844	-0.6701926660	0.0000000000
C	-0.6626084711	-1.8669729169	0.0000000000

H	0.0710858217	2.7371110924	0.0000000000
H	1.3025350231	1.8301503936	0.8820690048
H	1.3025350231	1.8301503936	-0.8820690048
H	-1.3221694878	0.7696536646	0.0000000000
H	1.2757567707	-0.8374049207	0.0000000000
H	-0.9153150858	-2.3766716032	0.9262556597
H	-0.9153150858	-2.3766716032	-0.9262556597

Butadiene

Energy: -156.001727 Ha

C	-12.1681419228	-3.6007707223	1.6484422843
C	-11.0643934186	-3.3446259168	2.3650859582
C	-9.7132120695	-3.6974293849	1.9463775663
C	-8.6093862991	-3.4407843723	2.6627762582
H	-13.1557299814	-3.3196279596	1.9997145745
H	-12.1157897475	-4.1014030516	0.6845399197
H	-11.1553956769	-2.8407740288	3.3276927107
H	-9.6223578103	-4.2023854271	0.9843356055
H	-8.6616203447	-2.9390149675	3.6260911964
H	-7.6217809655	-3.7217530827	2.3114068001

2,5-dihydrofuran

Energy: -231.225295 Ha

C	-12.1084343981	-3.6194047767	1.4398324524
C	-11.1325052004	-3.5825148860	2.3437532201
C	-9.7986522063	-3.5582101015	1.6482231518
H	-13.1751021685	-3.6454050989	1.6323856515
H	-11.2425098066	-3.5728238997	3.4223276681
C	-11.5174082998	-3.6227461182	0.0562746124
O	-10.1014900493	-3.5736143240	0.2506920155
H	-9.1765329103	-4.4303330469	1.9092176435
H	-9.2134216509	-2.6573705702	1.8950849816
H	-11.8441298228	-2.7560316651	-0.5412577434
H	-11.7892623336	-4.5283108816	-0.5109735082

2,5-dihydrofuran radical

Energy: -230.587931 Ha

C	-12.1217598526	-3.4799295295	1.4233614561
C	-11.0849164964	-3.5947368156	2.3354991013
C	-9.8989540410	-3.7173079296	1.6307445095
H	-13.1767281758	-3.3605730023	1.6238045374
H	-11.1647226977	-3.5925497583	3.4148252126
C	-11.5179666579	-3.5354159866	0.0521967153
O	-10.0930781683	-3.6882865693	0.2808228873
H	-8.8758920711	-3.8294779191	1.9589604502
H	-11.6708163887	-2.6237882415	-0.5485322450

H	-11.8577442185	-4.3881783916	-0.5585811484
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2,5-dihydrofuran-2-one

Energy: -305.269080 Ha

C	-12.1687138859	-3.5756911216	1.4344694009
C	-11.1921313869	-3.7048881109	2.3342837262
C	-9.8987673275	-3.8506713428	1.6176187060
H	-13.2298612533	-3.4504179295	1.6152950108
H	-11.2554087230	-3.7112148471	3.4136472236
C	-11.5707902614	-3.6293413694	0.0576314268
O	-10.1673600746	-3.8005595833	0.2641812341
O	-8.7849451556	-3.9900840989	2.0532370109
H	-11.7422805912	-2.7065615931	-0.5118425509
H	-11.9539556405	-4.4702401346	-0.5350875479

2,5-dihydrofuran-2-one radical

Energy: -304.632524 Ha

C	-12.1631644779	-3.5415165645	1.3941354760
C	-11.1867648138	-3.8380875176	2.3341705557
C	-9.9124873271	-3.9112692057	1.6530519478
H	-13.2242634097	-3.4139725943	1.5562758375
H	-11.2941722021	-4.0022041698	3.3958057081
C	-11.5161316302	-3.4314937900	0.1654699497
O	-10.1961307768	-3.6393234964	0.2639488233
O	-8.7794169065	-4.1351050006	2.0078516965
H	-11.9036798816	-3.2119064452	-0.8201080320

Carbene

Energy: -303.947400 Ha

C	1.1261202698	1.1357088079	0.0000000000
C	-0.2066123313	1.2214140008	0.0000000000
C	-0.7355403671	-0.1659911481	0.0000000000
O	0.4510253092	-1.0253519970	0.0000000000
C	1.5778973708	-0.3335987384	0.0000000000
O	-1.8342098877	-0.6220188256	0.0000000000
H	1.8404450720	1.9495351261	0.0000000000
H	-0.8665260854	2.0781090211	0.0000000000

Maleic anhydride

Energy: -379.289933 Ha

C	1.2855991629	-0.6976696086	0.0000000000
C	1.3166318284	0.6371887004	0.0000000000
C	-0.0905708610	1.1332661266	0.0000000000
O	-0.9294835408	0.0216032429	0.0000000000
C	-0.1431344929	-1.1278301430	0.0000000000

O	-0.5058966511	2.2569236321	0.0000000000
O	-0.6102079227	-2.2309880841	0.0000000000
H	2.1000649471	-1.4095271839	0.0000000000
H	2.1632738865	1.3104625640	0.0000000000

3.4 Optimized Intermediates: XI-VOPO₄ Slabs

The slabs are labelled according to figure S1. All coordinates are in angstroms.

3

Energy: -3.312994186779E+03 Ha

a = 9.36194256

b = 7.73512494

V	1.134958888474E-01	2.232938929843E+00	3.670303079732E+00
P	1.885606020210E+00	-5.018060651522E-01	3.416615557349E+00
O	1.241702506162E+00	-1.479058978536E+00	2.307515487794E+00
O	1.132572843637E+00	3.587677203058E+00	2.668384982824E+00
O	-4.235654288040E+00	-2.031682835414E+00	1.215578446790E+00
O	3.408892607128E+00	-3.068983195300E+00	2.932541218908E+00
O	5.817727608106E-01	2.629475066386E+00	5.226087764511E+00
O	1.278405328660E+00	8.974096985732E-01	3.081721479933E+00
V	-4.637997207420E+00	-1.845664625476E+00	2.705392375532E+00
P	2.607173983351E+00	3.668185046442E+00	1.923736601144E+00
O	3.330766785672E+00	2.266404595582E+00	2.187710743770E+00
O	3.456103886695E+00	-3.557308614094E-01	2.890685273711E+00
V	-2.008837005030E-01	-2.571348413678E+00	2.353141174781E+00
P	-1.928781815296E+00	6.247855124685E-02	2.614059534709E+00
O	-1.332739915962E+00	1.044651219136E+00	3.697204614765E+00
O	-1.236467010454E+00	3.713112494239E+00	3.291210902960E+00
O	4.143388034203E+00	1.592684718683E+00	4.678984561449E+00
O	-3.505746885665E+00	2.607499792760E+00	2.967194548484E+00
O	-5.971698636252E-01	-2.717212779071E+00	8.606132855931E-01
O	-1.309023068786E+00	-1.366011019459E+00	3.073417265227E+00
V	4.542409942781E+00	1.387909448512E+00	3.185785718721E+00
P	-2.722986863379E+00	3.605851283490E+00	3.977155015308E+00
O	-3.432957963806E+00	-2.722911540199E+00	3.721295198150E+00
O	-3.521861163184E+00	-1.046295891067E-01	3.047140433222E+00
O	1.818363659877E+00	-1.004474429930E+00	4.808813808174E+00
O	-2.681589589607E+00	3.201674666761E+00	5.392840558622E+00
O	2.524569383034E+00	-3.645051119000E+00	5.211344851374E-01
O	-1.733946990543E+00	4.150761721291E-01	1.197040830034E+00
C	1.240259752643E+00	3.825332538621E+00	5.825410299188E+00
C	1.374552638764E-01	-3.039598033651E+00	6.398239134580E+00
C	2.277310831350E+00	3.354032065556E+00	6.846001958067E+00
C	3.481570232576E+00	-3.425730467438E+00	6.843318032396E+00
H	4.160045915116E+00	-3.659923498757E+00	7.669300853441E+00

H 4.049043066660E+00 4.206683562611E+00 5.912918434479E+00
H 3.160070240500E+00 -2.381851855143E+00 6.932239554060E+00
H 2.606193292478E+00 2.341256143954E+00 6.599538042540E+00
H 1.809121868690E+00 -4.423545197936E+00 7.836733479599E+00
H 1.732719877006E+00 -3.416068898468E+00 4.984879762611E+00
H 6.092350006494E-01 -2.158507780256E+00 6.842493391307E+00
H -5.563596813911E-01 -2.699697846526E+00 5.626837091883E+00
H -4.245066349451E-01 4.142128819294E+00 7.155785018515E+00

6

Energy: -3.311757037206E+03

a = 9.36194256

b = 7.73512494

V 2.652642344973E-01 2.231156896747E+00 3.607573004613E+00
P 2.002262484524E+00 -5.315508425053E-01 3.373553222943E+00
O 1.405661301208E+00 -1.463746648688E+00 2.196056386779E+00
O 1.296782127008E+00 3.600548085072E+00 2.631408190041E+00
O -4.084372441001E+00 -2.039928894309E+00 1.237113779510E+00
O 3.569090124462E+00 -3.067289938367E+00 2.959103677363E+00
O 6.537805879846E-01 2.586333230116E+00 5.184940908181E+00
O 1.436269468277E+00 8.878000026112E-01 3.056549540377E+00
V -4.477787973177E+00 -1.848215542470E+00 2.728171914585E+00
P 2.790789510049E+00 3.664992007724E+00 1.937861535371E+00
O 3.491563893502E+00 2.258941870245E+00 2.244927302860E+00
O 3.599705309005E+00 -3.748793035193E-01 2.952656372266E+00
V -2.968263193437E-02 -2.568319481374E+00 2.274317111865E+00
P -1.805432664136E+00 5.129761079263E-02 2.527733462413E+00
O -1.180318695805E+00 1.044704489454E+00 3.574752670617E+00
O -1.071377151366E+00 3.717792557705E+00 3.227916530497E+00
O 4.311459583157E+00 1.576807759746E+00 4.741079413272E+00
O -3.355275411285E+00 2.606883957248E+00 3.015428880777E+00
O -4.172555423686E-01 -2.751406530339E+00 7.837322714486E-01
O -1.160233533425E+00 -1.369902407559E+00 2.971926140141E+00
V 4.696816617139E+00 1.380829158088E+00 3.241795085103E+00
P -2.527696189819E+00 3.616584036829E+00 3.969546765615E+00
O -3.266009746619E+00 -2.723753457776E+00 3.750051512795E+00
O -3.378928965982E+00 -1.128603356656E-01 3.047746302882E+00
O 1.818374683509E+00 -1.102065389957E+00 4.730714306301E+00
O -2.391697677693E+00 3.220682155008E+00 5.386070176556E+00
O 2.765522964634E+00 -3.670359219724E+00 5.265161600990E-01
O -1.695334365910E+00 3.814430692674E-01 1.097021301316E+00
C 8.306844239251E-01 3.757318725125E+00 6.098805113355E+00
C 2.023940331406E+00 3.518301694233E+00 6.945477198843E+00
C 3.195718436899E+00 4.113641266152E+00 6.680548285215E+00
C 4.442692406443E+00 3.930100751199E+00 7.483677272534E+00
H -4.114322684648E+00 3.527939031478E+00 6.855757159202E+00

H 4.796973666093E+00 -2.837325367028E+00 7.865110931932E+00
H 4.276400841561E+00 3.256014331124E+00 8.331054814805E+00
H 3.243884657612E+00 -2.944967459001E+00 5.827396206338E+00
H 1.922941687143E+00 2.830298525910E+00 7.782327871489E+00
H -1.258871672151E-01 -3.944200247995E+00 6.626702616153E+00
H 9.567234642975E-01 -3.102310283375E+00 5.455578603547E+00

8

Energy: -3.311109321866E+03 Ha

a = 9.36194256

b = 7.73512494

V 1.964923116866E-01 2.261518872416E+00 3.634100759558E+00
P 1.966558911191E+00 -4.746568366305E-01 3.327319774777E+00
O 1.303274704471E+00 -1.444891029021E+00 2.225460182547E+00
O 1.208409799361E+00 3.636091664527E+00 2.647528511146E+00
O -4.116299223799E+00 -2.024012141946E+00 1.188295485627E+00
O 3.487656503129E+00 -3.025982932648E+00 2.883156954145E+00
O 6.541893791378E-01 2.575433187198E+00 5.225363205440E+00
O 1.360608523191E+00 9.260400225414E-01 3.022089487168E+00
V -4.546803173969E+00 -1.817046868626E+00 2.667401228403E+00
P 2.673367236324E+00 3.715402535528E+00 1.883476608725E+00
O 3.402286533892E+00 2.311854965406E+00 2.135012620043E+00
O 3.534792076220E+00 -3.247005400874E-01 2.812795583424E+00
V -1.370390581996E-01 -2.545365449796E+00 2.315195779107E+00
P -1.861964052672E+00 9.467121509555E-02 2.548068087530E+00
O -1.262410890769E+00 1.081935369076E+00 3.620249294489E+00
O -1.157474256946E+00 3.763050623977E+00 3.307714378811E+00
O 4.201307932408E+00 1.628052528261E+00 4.620903674078E+00
O -3.432926179280E+00 2.651603155100E+00 2.915788825891E+00
O -5.585199181864E-01 -2.727363696846E+00 8.334985307050E-01
O -1.238577429855E+00 -1.327877871608E+00 3.024331738255E+00
V 4.611714603678E+00 1.430086363000E+00 3.128437315032E+00
P -2.658406043119E+00 3.630695459002E+00 3.953604845326E+00
O -3.361311080452E+00 -2.689211443239E+00 3.718119608674E+00
O -3.451481709406E+00 -6.977249173737E-02 3.000571896743E+00
O 1.904928939020E+00 -9.952507642276E-01 4.718211675486E+00
O -2.651144489580E+00 3.176339083498E+00 5.356131012083E+00
O 2.574578002756E+00 -3.602547470902E+00 4.805577800553E-01
O -1.684742939477E+00 4.243904768602E-01 1.124046597711E+00
C 1.041415896996E+00 -3.967235607680E+00 6.053647147701E+00
C -4.463772876026E-02 3.975855261928E+00 7.025943673351E+00
C -9.388904080691E-01 -2.682558109609E+00 7.040399611000E+00
C -8.684691395093E-01 -1.543516650927E+00 6.269352620013E+00
H 1.204622462806E+00 -3.135110150765E+00 5.368034420218E+00
H 1.992052741146E+00 -4.276947232244E+00 6.496872854228E+00
H -2.089867580290E-01 3.161527239854E+00 7.726749087899E+00

H -1.756613025167E+00 -2.764081707201E+00 7.752765312599E+00
H -5.561866799040E-02 -1.352431593547E+00 5.577476861290E+00
H -1.628518367716E+00 -7.749406076875E-01 6.373306970722E+00

9

Energy: -3.311149912899E+03 Ha

a = 9.36194256

b = 7.73512494

V -1.033381489951E-01 2.150893905755E+00 3.259625628225E+00
P 1.623298736941E+00 -6.106003621668E-01 3.310185598564E+00
O 1.017305320529E+00 -1.568025415633E+00 2.182884290238E+00
O 8.898348043208E-01 3.502879422976E+00 2.452312059654E+00
O -4.409210974913E+00 -2.129871674036E+00 1.224279098166E+00
O 3.174748948006E+00 -3.155529646281E+00 2.867918041848E+00
O 3.951392801405E-01 2.497439292735E+00 5.059121916287E+00
O 1.062023513982E+00 8.196365725570E-01 2.885623490949E+00
V 4.499032832435E+00 -1.937051753391E+00 2.701237265208E+00
P 2.475964841530E+00 3.602857565733E+00 1.748749280268E+00
O 3.085662302793E+00 2.211185787906E+00 1.992155187504E+00
O 3.193864194150E+00 -4.832775328516E-01 2.936785172226E+00
V -4.675626520264E-01 -2.618892825482E+00 2.169346705515E+00
P -2.274603225981E+00 -3.326938569569E-03 2.307025183095E+00
O -1.509154032579E+00 1.091726632568E+00 3.271220476380E+00
O -1.440122618161E+00 -3.977946787522E+00 3.141850689433E+00
O 3.804741017243E+00 1.592376359892E+00 4.694867953208E+00
O -3.737924524714E+00 2.675351147133E+00 2.890415848143E+00
O -8.294722018647E-01 -2.781346365091E+00 6.689446925587E-01
O -1.546438002823E+00 -1.339595693351E+00 2.817314359130E+00
V -5.100732524648E+00 1.325000399004E+00 3.205982250243E+00
P -2.937915287457E+00 -4.164347454628E+00 3.871311513837E+00
O -3.650482816073E+00 -2.709395484005E+00 3.777591346688E+00
O -3.734571348958E+00 -1.361163411323E-01 2.949377053998E+00
O 1.323406836696E+00 -1.030466434625E+00 4.705991301657E+00
O -2.709203698646E+00 3.144158602799E+00 5.273710367742E+00
O 2.347043870198E+00 -3.564050613014E+00 4.016872758945E-01
O -2.150466067504E+00 3.360089347593E-01 8.826673834191E-01
C 1.335564586610E+00 3.553036175065E+00 5.529132455633E+00
H 9.290957355316E-01 4.527125817634E+00 5.242023248195E+00
H 2.294161538481E+00 3.376602189901E+00 5.034481075698E+00
C -9.914300002698E-02 1.641112012529E+00 6.176200302255E+00
C 5.862220431980E-01 2.267396481300E+00 7.349459596343E+00
C 1.355531347431E+00 3.295313871696E+00 7.001140331162E+00
H 4.373059462581E-01 1.889133324049E+00 8.353975690523E+00
H 1.953336559761E+00 3.908153119224E+00 7.664843733951E+00
H 2.221229819058E-01 6.173158721985E-01 5.953067572753E+00
H -1.188416308472E+00 1.747771590745E+00 6.171394563409E+00

12

Energy: -3.385730582117E+03 Ha

a = 9.36194256

b = 7.73512494

V -6.056089915770E-01 2.489796790533E+00 4.829200090776E+01
P 1.149911401217E+00 -2.652695226747E-01 4.806023500509E+01
O 5.234150390895E-01 -1.223142001944E+00 4.692833566370E+01
O 4.104862554575E-01 3.847435811298E+00 4.727717682986E+01
O 4.438918265952E+00 -1.791128854374E+00 4.591865409628E+01
O 2.689668341937E+00 -2.814628109269E+00 4.760096137298E+01
O -1.966591329544E-01 2.806291937430E+00 4.985884776453E+01
O 5.633918637216E-01 1.139820678495E+00 4.773497251415E+01
V 4.006659037018E+00 -1.601975912448E+00 4.739932444477E+01
P 1.899430171552E+00 3.918188836689E+00 4.658406688379E+01
O 2.612808076678E+00 2.514647535890E+00 4.689382989121E+01
O 2.732771113772E+00 -1.154207722973E-01 4.757721362498E+01
V -9.218402784910E-01 -2.313739381398E+00 4.698654515617E+01
P -2.682710878167E+00 3.021327731531E-01 4.722549411764E+01
O -2.056686467698E+00 1.323058783060E+00 4.825268025672E+01
O -1.968406874162E+00 -3.757369032883E+00 4.791433620549E+01
O 3.386640242979E+00 1.806997780520E+00 4.939792019005E+01
O -4.248030844507E+00 2.864456534638E+00 4.770458770691E+01
O -1.318893367223E+00 -2.456883125133E+00 4.549410301664E+01
O -2.035054386549E+00 -1.105559980488E+00 4.770379113640E+01
V 3.805709099865E+00 1.633986624617E+00 4.790116594872E+01
P -3.417315698972E+00 3.871661085682E+00 4.865844361762E+01
O -4.156727604463E+00 -2.469439585639E+00 4.844977359437E+01
O -4.254536681439E+00 1.462959177424E-01 4.774156786306E+01
O 1.047225506132E+00 -7.967281156102E-01 4.944306165359E+01
O -3.293205869302E+00 3.463379985178E+00 5.007591848150E+01
O 1.878482472571E+00 -3.416023607974E+00 4.517296201232E+01
O -2.565803098748E+00 6.086090921091E-01 4.579034386972E+01
C -6.526738772103E-01 2.426288560642E+00 5.139480035725E+01
C 4.436700173831E-01 3.048623953480E+00 5.217777005286E+01
C 1.270431030461E+00 2.063941488289E+00 5.254486264193E+01
C 7.192349868198E-01 7.509191490054E-01 5.208140743580E+01
O -5.823319802440E-01 1.096588050242E+00 5.154027421986E+01
H 2.216750156245E+00 2.165772159125E+00 5.306257581640E+01
H 5.607471282534E-01 -3.617640726158E+00 5.229521409212E+01
H -1.670721098542E+00 2.811161726137E+00 5.133824373373E+01
H 5.504214046534E-01 2.724996397433E-02 5.288736367245E+01
H 1.305523420723E+00 2.787297933259E-01 5.128295449370E+01

13

Energy: -3.385848128173E+03 Ha

a = 9.36194256

b = 7.73512494

V -9.033515244163E-02 1.767016038500E+00 3.708366948648E+00
P 1.917435001648E+00 -9.136653681031E-01 3.702373348332E+00
O 1.200215123105E+00 -1.679650838060E+00 2.468381154440E+00
O 1.053003606649E+00 3.349061016340E+00 2.800051481729E+00
O -4.323359031124E+00 -2.234998607807E+00 1.239260302730E+00
O 3.395625882533E+00 -3.377694500042E+00 2.934073704374E+00
O 2.648831248184E-01 2.673771512002E+00 5.476264208118E+00
O 1.327839419099E+00 5.077791684441E-01 3.779518328000E+00
V 4.613957240680E+00 -2.140808396221E+00 2.735810384507E+00
P 2.494067023913E+00 3.299416235484E+00 1.991960402270E+00
O 3.120407343674E+00 1.922796789550E+00 2.324619242263E+00
O 3.433636223082E+00 -6.827750576331E-01 3.057602446711E+00
V -1.566897384156E-01 -2.862648245767E+00 2.471794282787E+00
P -1.858237471328E+00 -1.502186660375E-01 3.277541171489E+00
O -1.466638754546E+00 5.034809549073E-01 4.628359424712E+00
O -1.343599723266E+00 3.484683557592E+00 3.400265471662E+00
O 4.354361581304E+00 1.262142221768E+00 4.899186469885E+00
O -3.626478649808E+00 2.462766575845E+00 2.880579365119E+00
O -5.529699552815E-01 -2.982695261632E+00 9.765403522784E-01
O -1.309159371195E+00 -1.630567830755E+00 3.196277803817E+00
V 4.471436089967E+00 1.044517592941E+00 3.326115405658E+00
P -2.861800988526E+00 3.401230464661E+00 3.804687246299E+00
O -3.479837704668E+00 -2.895930300172E+00 3.834339874391E+00
O -3.426933875080E+00 -2.976800796309E-01 3.040329798256E+00
O 2.001131595303E+00 -1.729715257864E+00 4.939243533697E+00
O -2.872342664333E+00 2.918592267273E+00 5.317084188916E+00
O 2.388123416228E+00 3.767100943783E+00 6.014984266962E-01
O -1.113685454781E+00 8.216207740232E-01 2.297783880260E+00
C 2.852649320010E-01 3.738356408851E+00 6.111748054839E+00
C -6.152596535872E-01 -2.841030613365E+00 6.086377704750E+00
C -1.267053256620E-01 -1.934789438674E+00 6.941504040950E+00
C 1.112151687899E+00 -2.476754752726E+00 7.570516244886E+00
O 1.249169716990E+00 -3.801629479658E+00 7.014708538337E+00
H 1.063343314034E+00 -2.567076004497E+00 8.662140177794E+00
H 1.990834967508E+00 -1.900863461342E+00 7.264683761645E+00
H -5.123777664551E-01 -9.368648011586E-01 7.113614872859E+00
H -1.469990251163E+00 -2.729346716156E+00 5.446809864542E+00
H -3.552561871680E+00 2.222877980923E+00 5.461888091351E+00

16

Energy: -3.459728657160E+03 Ha

a = 9.36194256

b = 7.73512494

V -2.291806313290E-02 2.296677450497E+00 3.586524542013E+00

P 1.685599342731E+00 -4.784263383830E-01 3.336173258937E+00
 O 1.101482332756E+00 -1.403664263639E+00 2.143959537684E+00
 O 9.966371614490E-01 3.657412688378E+00 2.608222002483E+00
 O -4.395903876308E+00 -1.941867043092E+00 1.216552125496E+00
 O 3.264503170957E+00 -3.010592538691E+00 2.924633224384E+00
 O 4.818216720552E-01 2.680638597097E+00 5.145573827036E+00
 O 1.119241620152E+00 9.450947327057E-01 3.009545079470E+00
 V -4.785144271414E+00 -1.779920706808E+00 2.712793499331E+00
 P 2.493138134124E+00 3.718794148805E+00 1.902682680087E+00
 O 3.193823115034E+00 2.316816096997E+00 2.213996561524E+00
 O 3.288908188603E+00 -3.139626537378E-01 2.947343340483E+00
 V -3.401085986980E-01 -2.500159631854E+00 2.258546613034E+00
 P -2.100879339841E+00 1.320997950698E-01 2.560913918635E+00
 O -1.468594091321E+00 1.116480725311E+00 3.624569844155E+00
 O -1.368990745969E+00 3.779024381818E+00 3.208549850316E+00
 O 3.975072973386E+00 1.653814091758E+00 4.726554894016E+00
 O -3.655738319045E+00 2.667530208467E+00 3.024570997600E+00
 O -7.562183140160E-01 -2.682569682772E+00 7.756756168789E-01
 O -1.448636821471E+00 -1.293290341570E+00 2.981724701036E+00
 V 4.391814614356E+00 1.450291305709E+00 3.239702283058E+00
 P -2.824471732043E+00 3.689275135829E+00 3.968159655800E+00
 O -3.561444397009E+00 -2.655109742316E+00 3.704611543180E+00
 O -3.675225876874E+00 -4.095513235544E-02 3.061369463016E+00
 O 1.461641449604E+00 -1.066646625064E+00 4.678990489637E+00
 O -2.680504248169E+00 3.329785727614E+00 5.388548895261E+00
 O 2.452403125858E+00 -3.618545486009E+00 4.914880797234E-01
 O -1.968995629579E+00 4.962867194924E-01 1.139789019914E+00
 C 1.201610026146E+00 3.780618923632E+00 5.814879280362E+00
 C 1.844791808564E-01 -3.185384715099E+00 6.616500751223E+00
 C 4.664352057477E-01 -3.362332937268E+00 7.906282643773E+00
 C 1.668943457426E+00 3.504153527720E+00 8.021700823976E+00
 O 2.093206438356E+00 3.214116223108E+00 6.707617849783E+00
 H -5.444300952586E-02 -2.980829087582E+00 8.773913405214E+00
 H 1.716446980034E+00 -3.395253971046E+00 5.030256631050E+00
 H -6.265350153792E-01 -2.640061662703E+00 6.155285100186E+00
 O 2.252244843276E+00 3.085934270139E+00 8.975997970244E+00

17

Energy: -3.459813404642E+03

a = 9.36194256

b = 7.73512494

V -1.016992736821E-01 1.799595046946E+00 3.632259117971E+00
 P 1.885094289783E+00 -8.752820877351E-01 3.639868504702E+00
 O 1.194082597065E+00 -1.608476251062E+00 2.367915898569E+00
 O 1.048858187741E+00 3.408394857333E+00 2.711354228968E+00
 O -4.343990068819E+00 -2.170407618677E+00 1.201627633533E+00

O 3.390388136744E+00 -3.330692839424E+00 2.895250580067E+00
 O 4.058231083784E-01 2.771729664871E+00 5.353548893105E+00
 O 1.309009881914E+00 5.569143151239E-01 3.724630651709E+00
 V 4.606423845875E+00 -2.093298142187E+00 2.702902524989E+00
 P 2.502920457584E+00 3.347777451291E+00 1.934034212331E+00
 O 3.118142196412E+00 1.970665048588E+00 2.289382789196E+00
 O 3.422715547233E+00 -6.424276170864E-01 3.059397197984E+00
 V -1.549236376064E-01 -2.804241419133E+00 2.421523603779E+00
 P -1.857439113009E+00 -9.777981794915E-02 3.228244187164E+00
 O -1.470510152537E+00 5.949455790202E-01 4.565842083690E+00
 O -1.333766012084E+00 3.527402513377E+00 3.378650394449E+00
 O 4.350735845481E+00 1.325644819165E+00 4.866201884937E+00
 O -3.616898528177E+00 2.506206563206E+00 2.852677778223E+00
 O -5.966000309273E-01 -2.922012390040E+00 9.387323981298E-01
 O -1.291713950652E+00 -1.576823163762E+00 3.194643834508E+00
 V 4.468689832835E+00 1.095333587337E+00 3.298153965989E+00
 P -2.857169363847E+00 3.450111560084E+00 3.775256091601E+00
 O -3.474046522938E+00 -2.846763815371E+00 3.783460008329E+00
 O -3.424356759302E+00 -2.482960090474E-01 2.996362810292E+00
 O 1.884237965416E+00 -1.725595219548E+00 4.856985590014E+00
 O -2.865286680588E+00 2.987607574005E+00 5.292677591331E+00
 O 2.435256517985E+00 3.810958785956E+00 5.396615851979E-01
 O -1.095804832064E+00 8.523945040881E-01 2.233961162178E+00
 C 4.204951336629E-01 3.782403182954E+00 6.048037711941E+00
 C -5.448876542238E-01 -2.827306081230E+00 6.123756575486E+00
 C -6.652869694956E-02 -1.955855909701E+00 7.014849973758E+00
 C 1.207723394199E+00 -2.495038994891E+00 7.557847443894E+00
 O 1.416604773224E+00 -3.761502651366E+00 6.928473798056E+00
 H -4.653530696446E-01 -9.927431174875E-01 7.302801750199E+00
 H -1.428716433887E+00 -2.737124072172E+00 5.518740428178E+00
 H -3.557680179574E+00 2.310119281307E+00 5.462343654951E+00
 O 1.969399734441E+00 -2.078988549170E+00 8.371741460603E+00

3.5 Optimized Intermediates: α_1 -VOPO₄ Slabs

The slabs are labelled according to figure 3. All coordinates are in angstroms.

6

Energy: -1.733546330690E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.872710618556E+00 -1.661098992365E+00 1.093528316966E+00
 P -3.004448721099E+00 3.324732615172E+00 2.104489277376E+00
 O 2.989948267338E+00 2.041575955001E+00 1.273289022502E+00
 O -1.170871079920E+00 3.796260843769E-01 1.014814713891E+00

O 1.319626515322E+00 1.009413034426E-01 1.026775655250E+00
 O -4.810471649539E-02 -9.484200827420E-01 2.922514020887E+00
 O 1.938030351737E-01 1.516263943884E+00 2.881451163503E+00
 O -1.734694894943E+00 3.247248943876E+00 3.033742974190E+00
 O 1.875289600860E+00 -2.667177135609E+00 3.037970184659E+00
 V 7.168235159895E-02 3.372070824145E+00 2.498923041915E+00
 O 7.299267621725E-02 3.380814660142E+00 9.457522776279E-01
 V -2.991083011629E+00 1.871463525332E-01 1.452156015644E+00
 O -2.932047091567E+00 -3.464296827040E-02 3.176275909127E+00
 P 7.316812058120E-02 2.684110998454E-01 1.942672622287E+00
 C -3.095717118767E+00 7.637831605089E-01 4.356766162999E+00
 C -2.995776281066E+00 -1.128678717850E-01 5.559502547166E+00
 H 2.063327250376E+00 1.251299766402E+00 4.282057323596E+00
 H -2.327971410141E+00 1.544547070952E+00 4.366702897892E+00
 C -2.450244100924E+00 3.418007283981E-01 6.753801677041E+00
 H -3.373527840462E+00 -1.131025863265E+00 5.456803398795E+00
 C -2.438770842456E+00 -3.541247325994E-01 7.948637093228E+00
 H -1.997025963272E+00 1.334687848864E+00 6.743968198738E+00
 H 3.220422167904E+00 -1.323731507995E+00 8.053249035323E+00
 H -1.963173856922E+00 6.062746048237E-02 8.831056469398E+00

7

Energy: -1.733576807207E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.672791558018E+00 -1.817423305103E+00 7.473172820621E-01
 P -2.920089955146E+00 3.080631321231E+00 1.598521191858E+00
 O 2.977416851748E+00 1.824103459436E+00 7.710104033894E-01
 O -1.054038249230E+00 2.628912731597E-01 1.088781364017E+00
 O 1.378717325390E+00 -2.258824965752E-01 1.095862440099E+00
 O -3.607034155624E-02 -1.264804205815E+00 2.895762743626E+00
 O 3.422731845508E-01 1.307164618646E+00 2.896493178753E+00
 O -1.683543698697E+00 2.888887963853E+00 2.568906056841E+00
 O 1.982507145003E+00 -2.838885073308E+00 2.560171656677E+00
 V 1.478698031653E-01 3.093645560825E+00 2.236542890470E+00
 O 1.466001361594E-01 3.091871801075E+00 6.853295533720E-01
 V -2.899742837896E+00 -3.713822445043E-03 1.314331229026E+00
 O -2.909055777900E+00 -3.055778785801E-02 3.495362793141E+00
 P 1.628715863063E-01 1.968351047771E-02 1.987626646786E+00
 C -3.131587187278E+00 1.156834811667E+00 4.341596268821E+00
 C -3.170584522003E+00 6.412606670882E-01 5.740526362693E+00
 H 2.076913564700E+00 1.610748134534E+00 4.022800188532E+00
 H -2.306779331909E+00 1.847735027488E+00 4.177623661842E+00
 C -2.887666442612E+00 -6.535973141344E-01 5.769611077895E+00
 H -3.384071873743E+00 1.287316943341E+00 6.585433554768E+00
 C -2.660176968164E+00 -1.178721640683E+00 4.391832624258E+00

H -2.824841875450E+00 -1.293383626375E+00 6.643638807971E+00
H 2.778283326306E+00 -1.962363318325E+00 4.127611120567E+00
H -1.640171356287E+00 -1.516715164549E+00 4.221206902535E+00

10

Energy: -1.808172228686E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.940748542587E+00 -1.819526843333E+00 1.344099671482E+00
P -3.233262536021E+00 3.075004955673E+00 2.213155534221E+00
O 2.660570082625E+00 1.823775303227E+00 1.339455813568E+00
O -1.357235257949E+00 2.569253392807E-01 1.320847329550E+00
O 1.134721630692E+00 -2.871727269826E-01 1.419738815110E+00
O -4.044861818946E-01 -1.241825833063E+00 3.198022581493E+00
O 6.894176181985E-02 1.250506545937E+00 3.181004109461E+00
O -1.994855566115E+00 2.846705506586E+00 3.173553917011E+00
O 1.662566120042E+00 -2.826679403966E+00 3.156152894562E+00
V -1.821063715387E-01 3.075537308634E+00 2.717132110946E+00
O -1.835839987466E-01 3.079682423684E+00 1.166697158200E+00
V -3.177407441687E+00 4.164690708041E-03 1.855845505641E+00
O -3.070032125330E+00 4.718292698283E-02 3.528589861480E+00
P -1.437273664555E-01 -4.783000288331E-03 2.244020286930E+00
C -3.454704873874E+00 -3.707070051463E-02 4.918808130928E+00
C -3.003060043354E+00 -1.346211209784E+00 5.507662682714E+00
C -2.192980378581E+00 -1.084141516948E+00 6.527412637358E+00
H -3.310124723237E+00 -2.305463760045E+00 5.117990481688E+00
C -2.064242228218E+00 3.999452969804E-01 6.711306893673E+00
H -1.703686392969E+00 -1.805946279314E+00 7.172295627394E+00
O -2.801529424376E+00 9.689217515111E-01 5.620311951778E+00
H -1.029279696986E+00 7.624492021708E-01 6.710737709492E+00
H 3.610400148848E+00 7.318293357295E-01 7.655160648917E+00
H 1.609588865389E+00 1.605224992680E-01 4.895497646400E+00

11

Energy: -1.808197013461E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.900197434070E+00 -1.816408790740E+00 1.124360958783E+00
P -3.074155373473E+00 3.062854063013E+00 1.929189112020E+00
O 2.627878816430E+00 1.917573297445E+00 1.031157582802E+00
O -1.319569069508E+00 3.491098397414E-01 1.288561291694E+00
O 1.095189002879E+00 -2.682019380517E-01 1.243364689421E+00
O -3.634077029397E-01 -1.200508848433E+00 3.113307283853E+00
O 2.237399479376E-01 1.279940285281E+00 3.109011284449E+00
O -1.956181443073E+00 2.745577519284E+00 2.937221435067E+00
O 1.838545754037E+00 -2.856434186516E+00 3.074575820428E+00

V -1.225370016180E-01 3.107931171071E+00 2.432184081508E+00
O -7.211203555797E-02 3.134449934028E+00 8.676346070949E-01
V -3.189293109516E+00 5.498934937090E-02 1.324438399473E+00
O -3.227881888095E+00 1.913551268365E-01 3.323838246664E+00
P -9.570260744792E-02 4.080732863601E-02 2.193644913886E+00
H 1.897030339170E+00 2.475675893144E+00 3.622731318164E+00
C -2.955932575883E+00 -2.427638562844E-02 4.485653191515E+00
C -2.563838197534E+00 -1.260356693184E+00 5.184506146152E+00
C -2.425971231047E+00 -9.554693601408E-01 6.478421798031E+00
H -2.448977520203E+00 -2.207807816880E+00 4.678026446300E+00
C -2.706575973387E+00 5.053943491716E-01 6.684138419520E+00
H -2.146982070068E+00 -1.623088600486E+00 7.285847018784E+00
O -3.051366999293E+00 9.955555972511E-01 5.385121626011E+00
H -1.831093141422E+00 1.063105112788E+00 7.044405192154E+00
H 2.592055430759E+00 6.927959325803E-01 7.364159136228E+00

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Energy: -1.882119253115E+03 Ha

a = 6.14123848

b = 6.14323930

O -3.072091729574E+00 -1.704788022387E+00 1.005458209537E+00
P -3.321292775749E+00 3.224633944067E+00 1.933849532635E+00
O 2.647057223826E+00 1.952523336240E+00 1.073475517836E+00
O -1.495217206120E+00 3.059683862115E-01 1.066501335905E+00
O 9.917562643540E-01 -1.365197795909E-01 1.078986527353E+00
O -4.754858419640E-01 -1.131109215599E+00 2.920631475950E+00
O -3.417758450448E-02 1.314282718488E+00 2.933049079743E+00
O -2.047757945879E+00 3.074894700750E+00 2.869117462983E+00
O 1.659652986975E+00 -2.708950497507E+00 2.922995953686E+00
V -1.679987351753E-01 3.166499572953E+00 2.308625917001E+00
O -1.469208751229E-01 3.150056413054E+00 7.396408769536E-01
V -3.332732957086E+00 1.170251526517E-01 1.531450567596E+00
O -3.352315328679E+00 8.660469840303E-02 3.197875155374E+00
P -2.539762663979E-01 1.167397973060E-01 1.977655177896E+00
C 2.410691087614E+00 6.092094419854E-02 4.581020230541E+00
C 2.903701016175E+00 1.352346189822E+00 5.192750325977E+00
C -2.239987113803E+00 1.052559150699E+00 6.024658894343E+00
C -2.062467285529E+00 -4.245304125212E-01 6.050890789514E+00
O 3.116250881683E+00 -9.744720380215E-01 5.201980635801E+00
H 1.337464652716E+00 -1.348254246011E-01 4.595489420023E+00
H 2.521441811043E+00 2.320943884933E+00 4.896813161747E+00
H -1.629021338957E+00 1.733650953672E+00 6.603143289754E+00
O -1.300020264691E+00 -1.118167373009E+00 6.665140461853E+00

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Energy: -1.882219525989E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.636371765606E+00 -1.828858002143E+00 8.864069782066E-01
P -2.894265523834E+00 3.086540901703E+00 1.746615716050E+00
O 2.737810754071E+00 1.908643451448E+00 9.328717125669E-01
O -1.124600996850E+00 3.740840449396E-01 1.104524441830E+00
O 1.295517811132E+00 -3.128628046170E-01 1.078295439515E+00
O -1.839019438824E-01 -1.194929139729E+00 2.938532419589E+00
O 4.505764531474E-01 1.270057307943E+00 2.915635896518E+00
O -1.800264786551E+00 2.737346206902E+00 2.768373165539E+00
O 1.992172166095E+00 -2.671025262907E+00 2.795624909095E+00
V 5.062653418716E-02 3.090310944950E+00 2.276272943091E+00
O 6.842965756188E-02 3.108169538721E+00 7.104895707089E-01
V -2.981772861230E+00 4.740699923948E-02 1.144643435956E+00
O -3.055617146456E+00 -1.204983253490E-01 3.174299793354E+00
P 9.711752427367E-02 4.002207593171E-02 2.012282049741E+00
C 3.039390963918E+00 1.602188010754E-01 4.356701087602E+00
C 3.017540223796E+00 1.460721123157E+00 5.061811231704E+00
C -3.191591606255E+00 1.194190940923E+00 6.373051126186E+00
C -3.220574121485E+00 -2.800506065189E-01 6.557840806787E+00
O 2.967367519609E+00 -8.547617519900E-01 5.262671508029E+00
H 3.058361385248E+00 2.403763467117E+00 4.541978652266E+00
H -3.227491781716E+00 1.893161596676E+00 7.199542051235E+00
O -3.270008958099E+00 -9.699020697760E-01 7.532781447206E+00
H 2.086096002322E+00 -1.743170409651E+00 3.075653617225E+00

α_I -VOPO₄ after desorption, with missing vanadium oxygen

Energy: -1.502439124728E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.753939713875E+00 -1.903317067816E+00 8.615778006350E-01
P -2.966625845840E+00 3.033810306045E+00 1.807910499830E+00
O 2.962127996526E+00 1.827650701307E+00 8.615131188466E-01
O -1.146196810662E+00 1.558021476452E-01 1.382280839093E+00
O 1.355152430706E+00 -2.318040587980E-01 1.383214642585E+00
O -8.824149145162E-02 -1.324299604809E+00 3.156482722936E+00
O 2.959436646441E-01 1.248539875705E+00 3.156507468387E+00
O -1.746103425430E+00 2.822159813002E+00 2.777749986450E+00
O 1.953957296808E+00 -2.897962212811E+00 2.777613943241E+00
V 1.039095753501E-01 3.033743432845E+00 2.512086947921E+00
O 1.038934569401E-01 3.033746329973E+00 9.548543465692E-01
V -2.966265212333E+00 -3.773899655051E-02 1.024210181186E+00
P 1.041872605302E-01 -3.791377802514E-02 2.284497502320E+00

α_I -VOPO₄H after desorption, with missing vanadium oxygen

Energy: -1.503059333165E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.715903894772E+00 -1.943978741257E+00 8.420086990669E-01
P -2.909559042192E+00 2.978884566734E+00 1.737401730751E+00
O 2.802036807248E+00 1.798461869874E+00 8.652914333684E-01
O -1.185866208668E+00 2.043487021928E-01 1.457962522555E+00
O 1.337760786796E+00 -3.586530950585E-01 1.458820652078E+00
O -1.991423720774E-01 -1.325129856290E+00 3.227559275452E+00
O 3.833256640984E-01 1.214647846084E+00 3.199322015575E+00
O -1.836359972085E+00 2.660427637941E+00 2.785817109217E+00
O 2.027674223465E+00 -2.792570281066E+00 2.847781613372E+00
V 3.526381421232E-02 3.011662477461E+00 2.475861082743E+00
O 1.287526596720E-01 3.044294911184E+00 9.075023153697E-01
V -2.998984296418E+00 -7.173597225812E-02 1.095105702955E+00
P 7.910794973658E-02 -6.337144706406E-02 2.368964253717E+00
H 2.343177824611E+00 3.026686695961E+00 3.707901593780E+00

2-layer α_1 -VOPO₄

Energy: -3.155336642341E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.774924038499E+00 -1.856739404652E+00 1.039992259243E+00
P -2.967175319675E+00 3.033853924608E+00 1.962241845913E+00
O 2.981643327321E+00 1.781152222501E+00 1.040086980801E+00
O -1.149045762174E+00 1.544777029930E-01 1.039141975874E+00
O 1.355872774770E+00 -2.301007126279E-01 1.039104412109E+00
O -9.484086730156E-02 -1.285633400688E+00 2.872440478994E+00
O 3.017783176656E-01 1.210082408254E+00 2.872405440748E+00
O -1.719409924111E+00 2.835562886943E+00 2.873169158083E+00
O 1.926554132786E+00 -2.911079230049E+00 2.873464244820E+00
V 1.035300472429E-01 3.033893334905E+00 2.446214737393E+00
O 1.037853926760E-01 3.033978076511E+00 8.900662179152E-01
V -2.967190465282E+00 -3.777841153491E-02 1.485518434905E+00
O -2.967279080523E+00 -3.779027009734E-02 3.045207780520E+00
P 1.034533619209E-01 -3.776694628300E-02 1.961841099540E+00
O -2.767305109590E+00 -1.862431891011E+00 5.290991296137E+00
P -2.966031976079E+00 3.033653646756E+00 6.202590199596E+00
O 2.976613840598E+00 1.786491030849E+00 5.290989605306E+00
O -1.142262729899E+00 1.607300133672E-01 5.290229747550E+00
O 1.351599366970E+00 -2.365686992048E-01 5.290054304976E+00
O -8.811028614579E-02 -1.290185341268E+00 7.125055515972E+00
O 2.973451215789E-01 1.214193376084E+00 7.125198804902E+00
O -1.713951147038E+00 2.840977560227E+00 7.125856697619E+00
O 1.923350930175E+00 -2.916894009045E+00 7.126139290720E+00
V 1.046820915775E-01 3.033612685207E+00 6.681284538849E+00
O 1.049208008898E-01 3.033557026616E+00 5.121835623265E+00

V -2.965896140082E+00 -3.796911529891E-02 5.714568875517E+00
O -2.966032349793E+00 -3.798908027703E-02 7.270617532427E+00
P 1.047483753169E-01 -3.797012423852E-02 6.202242900306E+00

2-layer α_1 -VOPO₄ after desorption, with missing vanadium oxygen

Energy: -3.080132988561E+03 Ha

a = 6.14123848

b = 6.14323930

O -2.737002582705E+00 -1.860595387824E+00 1.057956609920E+00
P -2.964801588567E+00 3.030451287735E+00 1.985595117942E+00
O 2.949186346359E+00 1.776861925086E+00 1.060178312707E+00
O -1.147133780594E+00 1.860904592908E-01 1.048183678460E+00
O 1.361598973698E+00 -2.680251704677E-01 1.050110162328E+00
O -1.360387309226E-01 -1.282265399018E+00 2.873632737315E+00
O 3.480474068294E-01 1.201867030536E+00 2.874085818475E+00
O -1.724824895786E+00 2.792173678954E+00 2.889831688598E+00
O 1.936916493544E+00 -2.872504931434E+00 2.889725062180E+00
V 1.056874106087E-01 3.031791092434E+00 2.505134915289E+00
O 1.062610761537E-01 3.030749285446E+00 9.466513538413E-01
V -2.962734840386E+00 -4.209602361056E-02 1.469563881266E+00
O -2.959275582483E+00 -4.575903790224E-02 3.055851914976E+00
P 1.069676522982E-01 -4.024261063991E-02 1.975068058717E+00
O -2.631535763804E+00 -1.876858908973E+00 5.404833130275E+00
P -2.968731176262E+00 3.038418440493E+00 6.286982261476E+00
O 2.833835529135E+00 1.810790077599E+00 5.405017282513E+00
O -1.105531964579E+00 3.127014128211E-01 5.278879690354E+00
O 1.304024444491E+00 -3.802499755503E-01 5.275398178699E+00
O -2.040553094207E-01 -1.280737321231E+00 7.100508189852E+00
O 4.075503977405E-01 1.210256797971E+00 7.101803394579E+00
O -1.708977035522E+00 2.736772762034E+00 7.185525155698E+00
O 1.913327111201E+00 -2.805467314352E+00 7.187059979941E+00
V 1.024169592519E-01 3.036373024703E+00 6.703187607141E+00
O 1.043769426598E-01 3.034016717721E+00 5.135756569972E+00
V -2.972628934285E+00 -3.290914140527E-02 5.128033018199E+00
P 9.999479048729E-02 -3.448012870338E-02 6.175796229288E+00

3.6 Optimized Finite Cluster Transition States

The finite cluster transition states model those presented in figure 3 (and are labelled accordingly).

Modelling 1 to 2

V1	3.4850612703	3.1118159665	1.6602253413
V2	1.4844185994	3.5496732496	3.8822838008
V3	3.4861609361	1.2892420722	4.0639783117
P4	1.2113327458	1.1448293849	2.0702254828

O5	2.5440931450	2.5439163077	4.9139892104
O6	4.4379684448	2.1341802901	2.8108918468
O7	2.5498732112	4.2730010121	2.6458730016
O8	2.2336438596	0.4222526929	3.1120233867
O9	2.2179484468	1.9828464256	1.0949082356
O10	0.5273877766	2.3280971713	2.9625832491
O11	4.3228771463	3.7625101651	0.5060650141
O12	4.3286088217	0.3679638268	5.0136115437
O13	0.6185894560	4.5932598222	4.6710223472
O14	0.3354842946	0.2214159039	1.3207527856
C15	1.2664517792	-0.9454145055	-0.8080512454
C16	2.7350823772	-0.5136258362	-0.9490534338
C17	0.3926177293	-0.5750231478	-2.0076454856
C18	3.5227914036	-1.2369507563	-2.0492770778
H19	4.5628480874	-0.8946276387	-2.0932869507
H20	3.0768897160	-1.0656821495	-3.0345604740
H21	3.5325220822	-2.3193242922	-1.8751768161
H22	3.2484010271	-0.6734035168	0.0129747819
H23	2.7714582383	0.5713795476	-1.1301113041
H24	0.4260835349	0.5068984202	-2.1956909838
H25	-0.6546738493	-0.8421300954	-1.8267949349
H26	0.7027290912	-1.0771213043	-2.9333179017
H27	0.8206922593	-0.3838593832	0.2158893266
H28	1.2223680140	-2.0297137996	-0.6283812491

Modelling 3 to 4

P1	3.8768799528	2.4831408657	2.7811211481
P2	1.6330346881	3.8910453297	3.9652235419
P3	1.7251383649	0.9279727368	3.9612324562
V4	1.1683198212	2.2871910649	1.3653502106
O5	1.2531187337	2.4048633339	4.5360510436
O6	3.3060190941	1.2086090821	3.6481268068
O7	3.2049825521	3.7508165490	3.6010057245
O8	1.0576033420	0.8642917050	2.4996867219
O9	2.9889733664	2.4324912229	1.4549208631
O10	0.8789031380	3.8791000869	2.4490039353
O11	5.3314770925	2.5452128021	2.6752425506
O12	1.4514806174	-0.1748693661	4.8802999533
O13	1.2609326655	5.0008811353	4.8390821256
O14	0.7230272211	2.2132820266	-0.1378501730
C15	-1.6657849481	3.8696552917	2.9823645321
C16	-1.7513871559	2.4647900130	2.5896339921
H17	-2.1095764833	4.5888527192	2.2917747609
H18	-1.8624590282	4.0890207089	4.0293208773
C19	-1.6932450998	2.0117668858	1.2962416099
C20	-1.7541543381	0.5605910425	0.9154801057

H21	-1.4490430145	-0.0859448798	1.7425688373
H22	-1.1168931012	0.3497559520	0.0520948348
H23	-2.7799601066	0.2932952585	0.6282885787
H24	-1.6735488381	1.7183920725	3.3816094201
H25	-1.7939166278	2.7398882103	0.4921032406
H26	-0.4376468823	3.8857709586	2.7501638074

3.7 Optimized Constrained Slab Transition States

The transition states are labelled with respect to figure 3. All coordinates are in angstroms.

1 to 2

Energy: -3.313505794116E+03 Ha

a = 9.36194256

b = 7.73512494

V 2.549394664475E-01 2.150700199336E+00 3.363272343062E+00
P 2.221169411421E+00 -2.146902893935E-01 3.960922703856E+00
O 1.536586754511E+00 -1.599420213424E+00 3.613611102358E+00
O 1.389069253800E+00 3.593871448167E+00 2.823771949124E+00
O -4.380741313227E+00 -1.740020234658E+00 1.067125194983E+00
O 3.629717421233E+00 -3.006838165942E+00 2.895864600393E+00
O 8.274138193280E-02 2.077246845359E+00 4.909932379958E+00
O 1.409023249796E+00 8.352274381963E-01 3.022018535384E+00
V 4.796572914548E+00 -1.702117569806E+00 2.611487756094E+00
P 2.823349902321E+00 3.624987514398E+00 2.025137520067E+00
O 3.533587643159E+00 2.273003102859E+00 2.448661316640E+00
O 3.667864849851E+00 -2.662767854576E-01 3.190459630601E+00
V 1.477909479859E-01 -2.354080653902E+00 2.737941164586E+00
P -1.803053278507E+00 -3.081064879077E-03 2.120466057639E+00
O -1.135768827797E+00 1.383062127318E+00 2.512625900967E+00
O -1.008094204527E+00 -3.803785976583E+00 3.254842948667E+00
O 4.753934889821E+00 1.599731902258E+00 4.851755751843E+00
O -3.268470735345E+00 2.797699143130E+00 2.955095676084E+00
O 3.256949844431E-01 -2.233188177623E+00 1.198083856208E+00
O -1.022683454166E+00 -1.049273084206E+00 3.092595250995E+00
V -4.447614769646E+00 1.489898161799E+00 3.307839560988E+00
P -2.510801820832E+00 -3.858483823148E+00 3.879097306402E+00
O -3.178312657891E+00 -2.491935406742E+00 3.464136009026E+00
O -3.286385699584E+00 5.411620518249E-02 2.810002265584E+00
O 2.311284469643E+00 1.493641323655E-01 5.381409404504E+00
O -2.572380957211E+00 3.588633864664E+00 5.338200000000E+00
O 2.712443914531E+00 -3.829918955265E+00 5.883898467497E-01
O -1.820661494186E+00 -3.560791238368E-01 6.950365884823E-01
H -3.672783685714E+00 -3.831362085281E+00 6.153900000000E+00
C -4.616561115187E+00 -3.565196436095E+00 6.843300000000E+00
C -4.223258377403E+00 -2.402693085037E+00 7.753041041391E+00

C	3.538780571636E+00	-3.251377338407E+00	5.959372153786E+00
C	2.229498300918E+00	-3.081155606865E+00	6.745393934115E+00
H	-3.326798455939E+00	-2.638176641425E+00	8.337994055434E+00
H	4.335796677086E+00	-2.149343691273E+00	8.459756595445E+00
H	-4.017132967508E+00	-1.499857980855E+00	7.161151909581E+00
H	3.402922653483E+00	3.686623542874E+00	5.218877929743E+00
H	3.733924707288E+00	-2.324213707442E+00	5.399758941217E+00
H	2.014813229343E+00	3.747653499269E+00	7.323979533693E+00
H	1.382492411996E+00	-2.897488313736E+00	6.074353464356E+00
H	2.296185142520E+00	-2.233749088827E+00	7.434830170310E+00
H	4.543635878658E+00	3.262518140746E+00	7.431895984304E+00

3 to 4

Energy: -4.890045574451E+03 Ha

a = 6.14123848

b = 18.4297

O	-2.894721135885E+00	4.322358245597E+00	7.971588148828E-01
P	-3.009985842554E+00	3.020299693198E+00	1.654207568587E+00
O	3.057860872782E+00	1.836693285823E+00	6.456879767931E-01
O	-1.203370134435E+00	7.009819993039E-02	4.779986436502E-01
O	1.302902967234E+00	6.002040463926E+00	9.241956978178E-01
O	-5.105631846259E-02	4.823194551787E+00	2.743673696685E+00
O	1.360383548024E-01	1.180688712404E+00	2.385406543599E+00
O	-1.770535832214E+00	2.885422868855E+00	2.594743469702E+00
O	1.869988578545E+00	3.075970937619E+00	2.571921938066E+00
V	4.383243151257E-02	3.043106828195E+00	2.117790100435E+00
O	2.734595009383E-02	3.187569851251E+00	5.704772422494E-01
V	-3.016770610355E+00	6.089457803368E+00	1.398057965246E+00
O	-3.019452781007E+00	5.989978879612E+00	2.950749454319E+00
P	6.405362986907E-02	6.114462441207E+00	1.867461723627E+00
O	-2.972589773072E+00	-8.034936254253E+00	9.097122583139E-01
P	-2.990791659177E+00	9.204714814513E+00	1.896562344397E+00
O	2.974848063167E+00	7.925449951070E+00	1.036549222034E+00
O	-1.197071880294E+00	6.266450020463E+00	9.573197900720E-01
O	1.369313481265E+00	-6.250575364989E+00	4.911095695751E-01
O	2.628738118490E-02	-7.378044355057E+00	2.397336661638E+00
O	2.026093700395E-01	7.352035575182E+00	2.811817073383E+00
O	-1.700847662979E+00	9.135439280232E+00	2.771497480829E+00
O	1.925032613941E+00	-9.087869367000E+00	2.925900000000E+00
V	1.256696691424E-01	9.172750476630E+00	2.269479322170E+00
O	1.932794088363E-01	9.024413469556E+00	7.243136289524E-01
V	-2.934466181372E+00	-6.132835837212E+00	9.112948193019E-01
O	-2.843903757138E+00	-5.846812366404E+00	2.430536274405E+00
P	8.595914362596E-02	-6.206656401675E+00	1.367377291711E+00
H	2.195738406139E+00	-8.065758205000E+00	3.837600000000E+00
C	2.428368519762E+00	-7.191084643000E+00	4.620300000000E+00

C 1.595485880489E+00 -5.959428807714E+00 4.613452638538E+00
 C -2.708314994090E+00 -4.409029358548E+00 5.414237889787E+00
 H -1.943331896586E+00 -4.844365427077E+00 4.762141006374E+00
 H 3.604304602648E+00 -4.829072640286E+00 6.416806910033E+00
 H -2.643213465248E+00 -6.955645735154E+00 4.585391693404E+00
 H 2.267711552110E+00 -7.714447696256E+00 5.583192183300E+00
 O -2.994814601741E+00 -1.815040161447E+00 2.941161317002E-01
 P -2.999405245594E+00 -3.090755813983E+00 1.195245414881E+00
 O 3.165291626638E+00 -4.353810881993E+00 2.669470366068E-01
 O -1.140498215062E+00 -6.266921969573E+00 3.903381426910E-01
 O 1.298091563158E+00 -1.362154104669E-02 4.252026577623E-01
 O 5.190510048979E-02 -1.304517508749E+00 2.254524340226E+00
 O 2.516191931791E-02 -4.897399117774E+00 2.212557789174E+00
 O -1.769405612976E+00 -3.083297423608E+00 2.149820720067E+00
 O 1.884062569064E+00 -3.110091816117E+00 2.119678274737E+00
 V 5.977341574259E-02 -3.097704610076E+00 1.702219080183E+00
 O 5.121817842695E-02 -3.083454603085E+00 1.464931523739E-01
 V -3.027342826211E+00 -2.825229996221E-02 9.136648776794E-01
 O -3.042430799766E+00 -1.737663407514E-01 2.461194524079E+00
 P 6.551952393394E-02 -1.065914300711E-02 1.384338286445E+00
 C 2.039243904945E+00 -4.727313112610E+00 4.945622854756E+00
 H -2.542066124499E+00 -3.330629261482E+00 5.479031706190E+00
 H 1.328021802298E+00 -3.903805603983E+00 4.922005618218E+00
 H 5.473841715750E-01 -6.060689269332E+00 4.356150604796E+00